Plenary Lecture : **PLEN-1**
Plenary Lecture
Tamna Hall A THU 13:30
Chair: Tae-Lim Choi (Seoul National University)

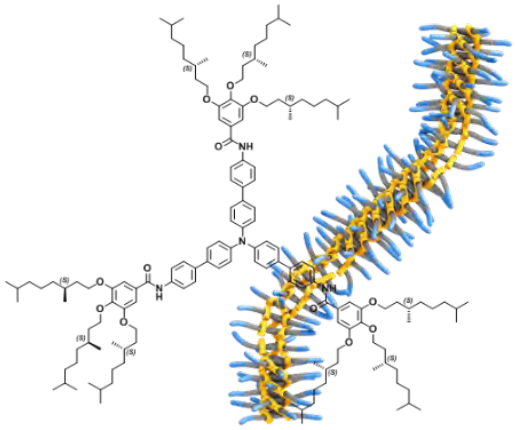
Functional Supramolecular Systems and Materials

E.W. Bert Meijer

Institute for Complex Molecular Systems, Eindhoven University of Technology, Netherlands

The intriguing prospects of molecular electronics, nanotechnology, biomaterials, and the aim to close the gap between synthetic and biological molecular systems are important ingredients to study the cooperative action of molecules in the assembly towards functional supramolecular materials and systems. For chemists, the non-covalent synthesis of these supramolecular architectures is regarded as one of the most challenging objectives in science: How far can we push chemical assembly processes, and can we get control over the properties and functions of the responsive and adaptive architectures made? Moreover, the increasing number of different components in the assembly processes increases the complexity of the system, as many competing events occur, and pathway selection is needed to arrive at the state required for the function. We therefore proposed a paradigm shift in synthetic chemistry, with the focus on non-covalent synthesis. [1] Mastering this complexity with a combination of experiments and simulations is a prerequisite to achieve the challenges set in creating functional materials and systems. In the lecture we illustrate our approach using some examples out of our own laboratories primarily based on the concept of supramolecular polymers. [2] In all cases the control over the position of the molecules in time and space is key to arrive at functionality.

[1] G. Vantomme, E.W. Meijer, Science 363, 1396-1397 (2019)
[2] T. Aida, E.W. Meijer, Israel J. of Chem. 60, 33-47 (2020)



Award Lecture : **AWARD1-1**

Award Lecture - 2022 KCS Excellence Academic Award

Tamna Hall A FRI 13:30

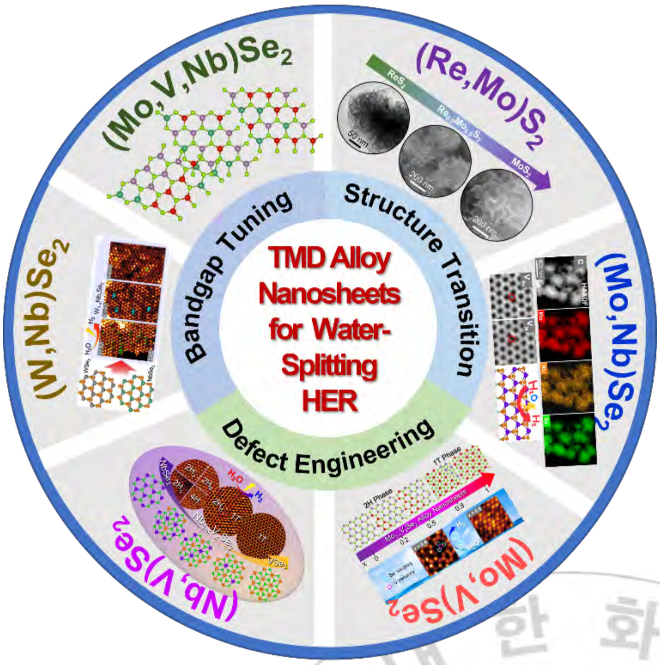
Chair: Taek Dong Chung (Seoul National University)

Two-Dimensional Transition Metal Dichalcogenide Alloy Nanosheets to Enhance Electrocatalytic Performance

Jeunghee Park

Department of Advanced Materials Chemistry, Korea University Sejong Campus, Korea

Semiconductor two dimensional nanostructures (nanosheets) have recently attracted considerable attention for many applications including electrochemical catalysts and flexible optoelectronic nanodevices. Phase control of nanosheets using alloy is challenging because of the band gap tunability as well as electronic structure modulation. We developed solution reaction method to synthesize alloy phase of group V-VI-VII transition metal dichalcogenide (TMD) nanosheets. The electronic structures were thoroughly examined using atomic resolution scanning transmission electron microscopy, X-photoelectron spectroscopy, and X-ray absorption spectroscopy. We observed that the alloying enhanced the electrocatalytic performance toward water-splitting hydrogen evolution reaction (HER). Extensive spin-polarized density functional theory calculations consistently predicted the alloy structures and the phase transition, in agreement with the experimental results. The Gibbs free energy along the pathway of HER indicates that the enhanced HER performance is correlated with the atomic structure of the alloyed nanosheets. Understanding the catalytic reaction at the atomic level would provide deep insight into the design of the energy conversion catalysts.


TMD Alloy Nanosheets for Water-Splitting HER
Bandgap Tuning
Structure Transition
Defect Engineering
(Mo,V,Nb)Se$_2$
(Re,Mo)S$_2$
ReS$_2$
MoS$_2$
(Mo,Nb)Se$_2$
(Mo,V)Se$_2$
2H Phase
1T Phase
(Nb,V)Se$_2$
(W,Nb)Se$_2$
H$_2$O
H$_2$

Symposium : **AWARD2-1**

Award Lecture - 2022 Man Jung Han Academic Award

Samda Hall WED 13:30

Chair: Gyochang Keum (KIST)

The Molecular Unflattening Project: Frustration, Adaptation, and Cooperation

Dongwhan Lee

Department of Chemistry, Seoul National University, Korea

Structure begets function. Novel functions emerge from novel structures, either by rational molecular design (as we often claim retrospectively even without guilt) or by sheer serendipity (although we ordinarily do not disclose). For some time now, my research group has been exploring the chemistry of bent and stackable polyaromatics as conformationally well-defined turn motifs for spontaneously folding π-conjugated molecules and self-assembling macrocycles.

What new properties would emerge if close π–π contacts between large and flat aromatic surfaces are intentionally thwarted? This open-ended question prompted our recent ventures into the chemistry of (i) porous crystals displaying cavity-changing motions, (ii) hydrophobic collapse of polycationic fluorophores, (iii) allosteric gating of canopied container molecules, (iv) sequence-specific interdigitation of molecular clips, and (v) hierarchical folding of cation-responsive molecular tweezers. This presentation will discuss key design principles, synthetic implementations, and functional consequences of the steric and electronic frustration that is endured (and also exploited) by triazoliptycenes, isobenzimidazoles, and even substituted benzenes.

Unflattening is about “restoring something flattened to its previous form” — or so they say. To me, it is seeing beauty hidden in plain sight, or even in sheer invisibility. That is where this title came from, “The Molecular Unflattening Project”, an unmatched liberating experience.

Symposium : **KCS1-1**

[Tutorial 1] NMR Spectroscopy in Natural Product Structure Elucidation

Tamna Hall B WED 15:00

Chair: Yunmi Lee (Kwangwoon University)

NMR Spectroscopy in Natural Product Structure Elucidation

Ki Hyun Kim

School of Pharmacy, Sungkyunkwan University, Korea

Nuclear magnetic resonance (NMR) spectroscopy is the most important technique used in the process of structure elucidation of organic natural products and chemical analysis of natural products. The tremendous development of sophisticated 1D and 2D-pulse techniques over the past three decades allows deep insights into the constitution, configuration, and conformation of complex organic molecules on a routine basis. The earlier bottleneck of low sensitivity and long measuring times resulting thereof has been eliminated by cryo-probes, higher field strengths, and fast acquisition techniques. The bottleneck nowadays can be found in the interpretation of the measured spectra despite the fact that sophisticated spectrum prediction and structure verification software is around.

This tutorial will show NMR data Interpretation of natural products by examples and exercises based on real NMR data including full one- and two-dimensional datasets of natural products. Advanced topics will include all of the common two-dimensional experiments (COSY, ROESY, NOESY, TOCSY, HSQC, HMBC) covered strictly from the point of view of data interpretation. In addition, this tutorial will introduce recent developed SMART NMR, which is an artificial Intelligence-based tool to generate structure hypotheses from NMR data.

Symposium : **KCS2-1**

[Tutorial 2] ABC Writing Skills: How Efficiently you can Write a Scientific Paper

Tamna Hall B WED 16:00

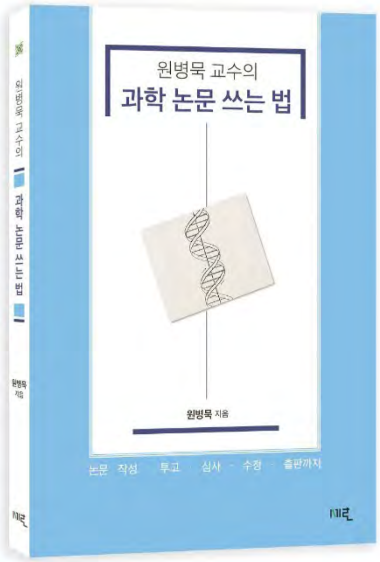
Chair: Tae Kyu Kim (Yonsei University)

ABC writing skills: how efficiently you can write a scientific paper

Byung Mook Weon

School of Advanced Materials Science and Engineering, Sungkyunkwan University, Korea

This lecture provides undergraduate and graduate students with the principles of 'how to write a scientific paper' and practically useful core writing skills. A practical 'ABC writing skill' is introduced. The most efficient paper writing is possible when the research results are achieved and well organized in figures and tables. The ABC writing skill is summarized as follows: A = After completing research, B = Based on well-organized figures and tables, and C = Compose logically a manuscript from a title to a conclusion.



Symposium : **KCS3-1**
[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications
Halla Hall WED 14:00
Chair: Sukwon Hong (GIST)

C-H Amidation Reactions via Metal-Nitrenoids: Mechanistic Studies and Asymmetric Catalysis

Sukbok Chang

Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea

Direct amidation of C–H bonds is a highly desirable reaction considering high utility of amidated products in total synthesis, medicinal chemistry and materials science. Although tremendous research efforts have been made especially in recent years, the current status enabling such C–H reactions in excellent stereoselectivity and high efficiency is still rather limited. In this context, we have developed a novel methodology that employs tailor-made Ir-based catalysts in combination with dioxazolone substrates to access a short-lived metal-nitrenoid intermediate, thereby eventually leading to a construction of γ-lactams via an outer-sphere C–H insertion pathway. The scope was found to be broad and a range of carboxylic acids could be readily utilized for the lactam formation. Indeed, the power of this new method was demonstrated in the successful late-stage functionalization of bio-active molecules to produce molecules that are highly sought after for pharmaceutical applications. More recently, we have successfully introduced an iridium-based catalyst system for asymmetric C−H amidation that enables facile construction of chiral γ-lactams starting from commodity chemicals. Various types of secondary C−H bonds, such as being positioned at the benzylic, unactivated aliphatic, propargylic, and allylic sites, were all smoothly reacted in a regio- and stereoselective manner. The present approach will find broad applications in medicinal chemistry, and the mechanistic insights may provoke further developments in related asymmetric catalysis.

Symposium : **KCS3-2**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 14:20

Chair: Sukwon Hong (GIST)

P^N ligands in the Ni-Catalyzed Reactions of Alkynes

Eun Jin Cho

Department of Chemistry, Chung-Ang University, Korea

The use of Ni(II) complex with bidentate P^N ligands showed excellent reactivities in the reactions of alkynes. The Ni/P^N system has the potential to undergo transmetalation with boronic acid derivatives followed by arylative nickelation of alkynes to give alkenyl Ni-intermediate which can act as nucleophile reacting with carbonyls. Multi-functionalized polycyclic heterocycles including benzofuran, indole, and isoindoloindolone systems have been synthesized from alkyne-tethered carbonyl derivatives. On the other hand, Ni(0)/P^N has ability to undergo oxidative cyclizations with two pi systems to form a five membered Ni(II) nickelacycle intermediate. A synthetic route for accessing multifunctionalized indoles was developed through Ni(0)-catalyzed transcarboamination using 2-alkynylanilinoacrylate. In addition, this Ni(0) chemistry could be utilized for an exogenous base-free procedure of a stereoselective arylvinylation of alkynes with boronic acids affording tetrasubstituted 1,3-diene products stereoselectively.

Symposium : **KCS3-3**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 14:40

Chair: Sukwon Hong (GIST)

Understanding Photoredox Chemistry – Insights from Computer Models

Mu-Hyun Baik

Institute for Basic Science (IBS) & KAIST, Korea

Using photoredox chemistry to in situ prepare reactive intermediates that are not accessible through other more traditional means has become a method of choice for many organic reactions. Recent advances have shown that these photochemically induced reactions can show exquisite regio- and stereochemistry. The active intermediates of these reactions are exceedingly difficult to characterize or study in detail, as the reactions are typically too fast. Computational models offer an attractive alternative, but there are methodological challenges to overcome. In this presentation, I will discuss what we learned in the recent past about these reactions.

Symposium : **KCS3-4**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 15:00

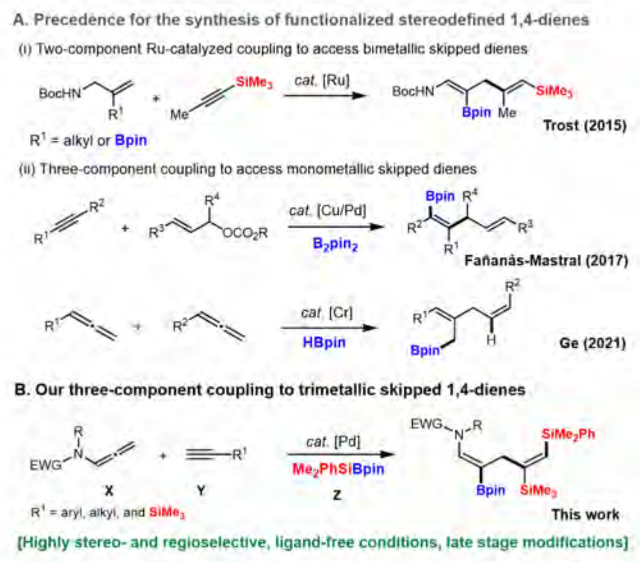
Chair: Sukwon Hong (GIST)

Silaborative Assembly of Allenamides and Alkynes: Highly Regio- and Stereoselective Access to Bi- and Trimetallic Skipped (Z,Z)-Dienes

Jin Kyoon Park

Department of Chemistry, Pusan National University, Korea

While multi-component coupling reactions are successful in regio- and stereoselective assemblage, incorporation of metallic group in skipped dienes is scarce. For instance, Trost group reported pioneering work on Ru-catalyzed two-component alkene-alkyne coupling in 2015.[1a] Relevant to a three-component coupling approach, Mastral group discovered a synergistic copper/palladium catalytic system to couple allyl carbonate and alkyne with bis(pinacolato)diboron (B_2Pin_2) (top, Scheme A(ii)).[1b] Ge group has also reported an elegant atom-economic catalytic method to access boryl-functionalized (E,Z)-1,4-dienes by taking advantage of a chromium(I) hydride intermediate (bottom, Scheme A(ii)).[1c] To our knowledge, however, analogous coupling strategies between two types of electronically-differentiated C−C π systems employing unsymmetrical interelement reagents (e.g. [Si]-[B]) remain unknown. Herein, a highly stereo- and regioselective multicomponent approach to access (Z,Z)-skipped 1,4-dienes decorated with silyl and boryl functionalities has been described.[2] This Pd-catalyzed orchestrated atom economy union proceeds without the use of phosphine ligand via a neighboring amide group chelation. A variety of alkynes, as well as allenamides, could be employed to react with $Me_2PhSi{-}Bpin$ in good yield and excellent selectivity. AcknowledgementThis study was supported financially by the National Research Foundation of Korea (NRF) (2012M3A7B4049644, 2019R1A2C2004902, 2019R1A4A1028007) References1.(a) Trost, B. M.; Cregg, J. J. J. Am. Chem. Soc. 2015, 137, 620. (b) Mateos, J.; Rivera-Chao, E.; Fañanás-Mastral, M. ACS Catal. 2017, 7, 5340. (c) Zhao, Y.; Ge, S. Angew. Chem. Int. Ed. 2021, 60, 2149.2.Angew. Chem. Int. Ed. 2022, 10.1002/ange.202116154


A. Precedence for the synthesis of functionalized stereodefined 1,4-dienes
(i) Two-component Ru-catalyzed coupling to access bimetallic skipped dienes
BocHN
R1
+
SiMe3
Me
cat. [Ru]
BocHN
Bpin
Me
SiMe3
Trost (2015)
R1 = alkyl or Bpin
(ii) Three-component coupling to access monometallic skipped dienes
R1
R2
+
R3
R4
OCO2R
cat. [Cu/Pd]
B2pin2
Bpin
R4
R2
R1
R3
Fañanás-Mastral (2017)
R1
+
R2
cat. [Cr]
HBpin
R1
Bpin
R2
H
Ge (2021)
B. Our three-component coupling to trimetallic skipped 1,4-dienes
R
EWG
N
X
+
R1
Y
cat. [Pd]
Me2PhSiBpin
Z
EWG
N
R
SiMe2Ph
Bpin
SiMe3
This work
R1 = aryl, alkyl, and SiMe3
[Highly stereo- and regioselective, ligand-free conditions, late stage modifications]

Symposium : **KCS3-5**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 15:40

Chair: Eun Jin Cho (Chung-Ang University)

Chemically Recyclable Functional Polymers Enabled by Ring-Opening Metathesis Polymerization with Elaborately Designed Catalysts and Monomers

Soon Hyeok Hong

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The development of chemically recyclable polymers is a critical challenge for a sustainable future. Our group has made continuous efforts to identify suitable catalysts and develop novel polymerization methods to address the challenge. Herein, we present novel chemically recyclable polymers with high oxygen barrier properties and hydrolytic stability synthesized by the elaborate design of monomers and catalysts. The obtained polymers could be recycled by strategical chemical transformations, demonstrating that both open-loop and close-loop recycling is possible with the designed material.

Symposium : **KCS3-6**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 16:00

Chair: Eun Jin Cho (Chung-Ang University)

Fascinating Construction & Restructure of Heterocyclic Compounds via Dearomative Strategies

Eun Jeong Yoo

Department of Applied Chemistry, Kyung Hee University, Korea

Heterocyclic compounds found in numerous natural products are an important class of structural motifs. Their potent biological activities and interesting medicinal effects have an impact on the pharmaceutical industry. [m+n] dipolar cycloaddition is a powerful and widely used strategy as it ensures 100% atom economy with a single operation. Along with cycloadditions, the restructuring of ring skeletons, such as contraction, expansion, deconstruction, and fusion, is also an efficient and prevalent method to achieve molecular diversity. In this seminar, we will discuss the construction and restructure of N-heterocyclic compounds using atypical N-aromatic zwitterions. First, a catalytic ring-expansion of N-aromatic zwitterions through 1,4-dearomative addition of diazoacetates will be presented for the construction of various fused azepines by an elaborate control of the reaction kinetics at each step. Next, we will describe the valence tautomerization of fused 1,4-diazepines, which reconstructs pyrrole derivatives and releases HCN gas. Several factors that influence the equilibrium between each valence tautomer of an 8π-electron diazepine skeleton will be explained. In addition, we will introduce an unprecedented strategy for the cycloadditive ring-contraction of N-aromatic zwitterions and alkynes is developed to afford aryl- or alkyl-substituted pyrrolo[1,2-a]quinolines that were otherwise challenging to fabricate.

Symposium : **KCS3-7**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 16:20

Chair: Eun Jin Cho (Chung-Ang University)

Regio- and Enantioselective Alkene Functionalization

Sungwoo Hong

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Catalytic alkene functionalization is a powerful synthetic tool for the direct installation of functionalities across alkenes to enable the rapid buildup of molecular complexity from abundant and readily available alkenes. Chemical methods to achieve this goal could have broad application potential in synthetic organic chemistry, considering the reduction in the number of synthetic steps and the abundance of inexpensive starting materials. For example, forming asymmetric C–N bonds from various alkenes via a direct catalytic method is a powerful way of synthesizing value-added chiral amines. Presented in this symposium are our investigation of regio- and enantioselective alkene functionalization under Ni-catalyzed or photochemical conditions. These new catalytic synthetic methods allow us to perform the unprecedented disconnection of target molecules, affording innovative and imaginative synthetic strategies of so-called "privileged scaffolds". These new catalytic synthetic methods will function as competent tools directly utilized in cross-coupling reactions capable of connecting privileged building blocks, providing opportunities for the successful implementation of fragment-based drug design (FBDD), and eventually streamlining drug discovery research.

Symposium : **KCS3-8**

[IBS Symposium] Frontiers in Developing Catalytic Organic Reactions and Investigating Their Applications

Halla Hall WED 16:40

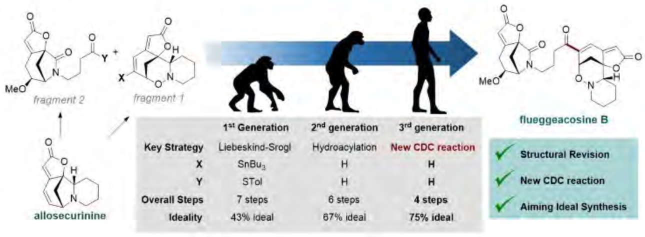
Chair: Eun Jin Cho (Chung-Ang University)

Synthesis of flueggeacosine B: Biosynthetic insights, structure revision, and development of the catalytic cross-dehydrogenative coupling reaction

Sunkyu Han

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

“Complex natural products serve as a source of inspiration for the development of new synthetic methods” has been a widely used cliché in the synthetic chemical community. However, in reality, even the most innovative total synthesis papers are made up of strategic composition and ingenious applications of “existing methods”. “Natural products-inspired methods development” is simply hard. Herein, we present our synthetic journey toward flueggeacosine B, a dimeric securinega alkaloids, that involved an actual invention of a new synthetic method. The structure of flueggeacosine B urged us to develop a polarity mismatched cross-dehydrogenative coupling (CDC) reaction between aldehyde and electron deficient olefin, a historically elusive transformation. We responded to the challenge by inventing a visible-light-mediated copper-catalyzed CDC reaction that consists of a hydrogen atom transfer and an oxidation of electron deficient radical. This discovery enabled us to complete the synthesis of flueggeacosine B in 4 overall steps from readily available allosecurinine (75% ideality based on Baran’s ideality measure).



	1st Generation	2nd generation	3rd generation
Key Strategy	Liebeskind-Srogl	Hydroacylation	New CDC reaction
X	$SnBu_3$	H	H
Y	STol	H	H
Overall Steps	7 steps	6 steps	4 steps
Ideality	43% ideal	67% ideal	75% ideal

✓ Structural Revision
✓ New CDC reaction
✓ Aiming Ideal Synthesis

Symposium : **KCS4-1**
[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions
Samda Hall WED 14:30
Chair: Hye Ryung Byon (KAIST)

Heterogeneous Electron Transfer Kinetics at the Inner Helmholtz Plane between Polybromide and Platinum

Taek Dong Chung

Department of Chemistry, Seoul National University, Korea

Strong electric field in the electric double layer of electrode-electrolyte interface offers unique environment for electrochemical reactions. Yet, it is challenging to evaluate physicochemical properties of the matter within the electric double layer. The impact of interfacial electric field is more prominent in room-temperature ionic liquids in which charge density of the electric double layer is much higher than that of conventional electrolytes. Recent approaches on this topic employed the linker molecules to make the redox species anchored onto the electrode. However, it cannot access the properties of the inner Helmholtz plane, where most of electrochemical reactions occur under the strongest electric field. The inner Helmholtz plane is extremely thin nano-space over the electrode surface, which has not allowed to be experimentally explored before. In particular, reorganization energy is the governing descriptor that would explain heterogeneous electron transfer kinetics and mechanism of coupled processes. Unfortunately only a few studies to measure reorganization energy in the inner Helmholtz plane has been done so that electrocatalytic activities in ionic liquids remain unclear. In this talk, I introduce a new way to determine the reorganization energy of Br2 reduction in a redox-active ionic liquid, 1-ethyl-1-methylpyrrolidinium polybromide (MEPBr2n+1). Exceptionally fast mass transport of Br2 in MEPBr2n+1 enables that the rate of electron transfer, not mass transport, controls the current in the MEPBr2n+1. And I discuss how sensitive the reorganization energy in the inner Helmholtz plane is to the surface charges of the electrode, suggesting the effect of potential zero charge and polarizability of the medium.

Symposium : **KCS4-2**

[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions

Samda Hall WED 14:45

Chair: Hye Ryung Byon (KAIST)

Symmetry-adapted Synthesis of Tailor-made Dicopper Oxidases with Diverted Dioxygen Reactivity

Woon Ju Song

Department of Chemistry, Seoul National University, Korea

Numerous dinuclear metalloenzymes show structures and functions distinct from mononuclear metal-containing enzymes, and their reactivities are further diverged by altering the distance between two metal ions. We are interested in creating artificial dinuclear metalloenzymes with structural accuracy and functional diversity to feed our understanding of enzyme emergence, evolution, and divergence. Thus, we herein genetically incorporated a Cu-binding site per protomer in the vicinity of the innate rotational axis of a homohexameric protein. The inherent protein symmetry operation multiplies metal-binding moieties, resulting in various artificial mononuclear or dinuclear copper-binding proteins. Consequently, they displayed multiple reactivities with dioxygen associated with two or four protons/electrons, resembling the divergent evolution of the shared active sites for a diverse chemical repertoire of artificial copper-dependent oxidases.

Symposium : **KCS4-3**
[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions
Samda Hall WED 15:00
Chair: Hye Ryung Byon (KAIST)

Interface structure-electrocatalytic activity/stability relationship

Chang Hyuck Choi

Department of Chemistry, Pohang University of Science and Technology, Korea

Electrochemical energy conversion has been recognized as a promising strategy for pursuing a sustainable energy society. In this new energy scenario, electrocatalysis becomes a key technology enabling efficient energy conversion between chemicals and electricity. In the past few decades, significant efforts have been made to improve catalytic performance solely by modification of catalytic materials (e.g., doping, alloying, morphological engineering, etc.), which has successfully led to remarkable advances in initial catalytic activity. Beyond materials engineering, solid-liquid interface engineering, i.e., electrode-electrolyte interfaces (e.g., electric fields, solvents, reactants, pH, cationic species, etc.), has recently been considered for better electrocatalysis, but the understanding of the underlying fundamental mechanism is highly missing. Here we show our recent findings that the nature and concentration of ionic species in electrolytes play critical roles in electrocatalysis. On the one hand, we demonstrated that the cation-coupled electron transfer (CCET) step, along with two common electron transfer mechanisms in aqueous electrolytes (electron transfer (ET) and proton-coupled electron transfer (PCET)), is available under certain conditions. The CCET mechanism, whose kinetics is affected by cation identity and concentration, governs overall electrocatalysis. On the other hand, we revealed that electrocatalytic stability can also be affected by the chemical properties of the electrode-electrolyte interface. Electrochemical CO_2 reduction and Pt dissolution were used here as model reactions to explain the so-called ‘cationic effects’.

Symposium : **KCS4-4**

[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions

Samda Hall WED 15:15

Chair: Hye Ryung Byon (KAIST)

Unusual Chemistry Induced by Plasmonic Hot Electrons

Zee Hwan Kim

Department of Chemistry, Seoul National University, Korea

The plasmonic hot electrons, the high-energy electrons of metallic nanoparticles created by the non-radiative decay of plasmon oscillation, is known to induce highly exotic chemical reactions that no other heterogeneous (photo) catalysts can offer. However, the underlying mechanism is largely unverified thus far. In this talk, I will present my research group's recent endeavor to uncover the mechanism of hot-electron induced chemical reactions, and to expand the scope of the reaction.

Symposium : **KCS4-5**

[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions

Samda Hall WED 15:30

Chair: Hye Ryung Byon (KAIST)

Synthetic Control of Photoinduced Electron Transfer of Transition Metal Complexes

Youngmin You

Chemical Engineering and Materials Science, Ewha Womans University, Korea

Photoredoxcatalysis emerges as a promising strategy for organic radical transformations because it can be executed under mild reaction conditions and is amenable to a wide range of substrates. The photoredoxcatalysis requires photoactive catalysts with high redox stability and large driving forces for the redox mediation. Cyclometalated complexes of Ir(III) and Pt(II) meet these criteria, as their strong cyclometalation enables wide tunability in structural and electrochemical properties. My group has been involved in continued effort toward understanding and maximizing photoredoxcatalysis ability of the metal complexes. We are particularly interested in deciphering excited-state behaviors, including back electron transfer as well as the forward electron transfer, based on transient spectroscopic, electrochemical and quantum chemical techniques. Our mechanistic studies have provided valuable insight into designing of photoactive cyclometalated complexes with enhanced catalytic properties.

Symposium : **KCS4-6**
[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions
Samda Hall WED 15:50
Chair: Hye Ryung Byon (KAIST)

Ionovoltaic Analysis and Engineering

Youn Sang Kim

Chemical and Biological Engineering, Seoul National University, Korea

Recently, various energy transducers driven by the relative motion of solids and liquids have been demonstrated. However, in relation to the energy transducer, a proper understanding of the dynamic behavior of ions remains unclear. Moreover, the energy density is low for practical usage mainly due to structural limitations, a lack of material development stemming from the currently poor understanding of the mechanisms, and the intermittently generated electricity given the characteristics of the water motion (pulsed signals). Here, we demonstrate a method by which to generate continuous electrical energy with the flow of a water droplet through an electrolyte-insulator-semiconductor (EIS) structure. The output power and energy conversion efficiency of the transducer are 29.8 %. Also, we propose and verify a hypothesis pertaining to the ion-dynamic operation mechanism of the transducer, "ionovoltaic" device, which holds that the electron flow is induced by ions. Further, we describe ion specificity and bio-sensing fuctionality, an important characteristic of electrical signals generated by various water motion, in relation to the potential profile of electric double layer, which is determined by the characteristics of microscopic ion properties. This presentation will present the possibility of a new concept device to researchers in the field of energy harvesting, and provide insight in various fields such as electrochemistry, life science, and colloidal engineering with a new perspective on the behavior of ions at the solid-liquid interface.

Symposium : **KCS4-7**

[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions

Samda Hall WED 16:10

Chair: Chang Hyuck Choi (POSTECH)

Data-driven multiscale models to understand electrochemical reactions

Yousung Jung

Department of Chemical & Biomolecular Engineering, Korea Advanced Institute of Science and Technology, Korea

Understanding chemical reactions at the electrochemical interfaces is challenging due to the multiscale nature of the phenomena, theoretical descriptions of which would require the prediction of adsorbate binding, effects of potential, solvation, kinetics, and etc. In this talk, I will present some of our recent efforts to understand electrochemical reactions such as nitrogen reduction, hydrogen evolution, and carbon dioxide reduction reactions, by combining machine learning and multiscale strategies. We present a simple and versatile representation, applicable to any deep-learning models, to predict the binding energy of small molecules, and apply the model to study the extraordinary mass activity of jagged Pt nanowires toward hydrogen evolution reaction. Effect of potential is demonstrated to be critical to properly understand several electrochemical reactions.

Symposium : **KCS4-8**
[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions
Samda Hall WED 16:25
Chair: Chang Hyuck Choi (POSTECH)

Cation Effects on Oxygen Evolution Reaction using LiCoO2 Catalysts

Hye Ryung Byon

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Oxygen evolution reaction (OER) has been extensively investigated using various 3d-block transition metal oxide catalysts. In particular, the cobalt ion was widely incorporated and afforded reasonable OER activity. However, the specific active sites have been still debated. Regarding different local and bulk oxide structures, Co2+, Co3+, and Co4+ were proposed as the active cores. In recent, LiCoO2, which has been known to a positive electrode in lithium-ion batteries, was spotlighted as a new class of OER catalyst. The oxidation of Co3+ is accompanied by extraction of Li+, which induces local and bulk structure change of Li1-xCoO2. The previous report demonstrated the altered oxide structure from two-dimensional layer to monoclinic crystal after eliminating 0.5 Li, where Co4+ was presumed to be the active OER site.[1] The spinel LiCoO2 was higher activity than the layered one, revealing that the crystalline structure determines the OER activity.[2] Herein, we show the other important effect, electrolyte cation, for OER activity. The different cations of Li+, Na+, K+ and Cs+ from the alkaline electrolyte solutions alter OER activity and stability of Li1-xCoO2. I will present the role of electrolyte solutions using diverse in situ and ex situ characterizations and suggest the presumable active sites of the Li1-xCoO2 catalyst in this presentation. References[1] Z. Lu et al., J. Am. Chem. Soc. 2017, 139, 6270-6276[2] T. Maiyalagan et al., Nat. Commun. 2014, 5:3949

Symposium : **KCS4-9**

[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions

Samda Hall WED 16:40

Chair: Chang Hyuck Choi (POSTECH)

Visible-light Driven RAFT Polymerization

Min Sang Kwon

Department of Materials Science and Engineering, Seoul National University, Korea

Photomediated-RAFT has recently received great attention due to its unique features such as oxygen tolerance, excellent monomer compatibility, and applicability to the synthesis of high molecular weight polymers. In this talk, I will summarize current development of photomediated-RAFT polymerization and also introduce our approaches for visible-light driven RAFT polymerizations.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **KCS4-10**

[SNU-SRC Symposium] Frontiers of Electron Transfer Chemical Reactions

Samda Hall WED 16:55

Chair: Chang Hyuck Choi (POSTECH)

To Transfer, or Not To Transfer, That is the Question: Designer Hydrogen Bonds for Biomimetic Electron Transfer

Dongwhan Lee

Department of Chemistry, Seoul National University, Korea

Chemistry is about making and breaking bonds by redistributing electron densities between the nuclei. While there should be no apparent dichotomy in this general understanding, anything that is non-covalent is often unjustifiably relegated to the periphery and classified simply as "secondary". However, numerous examples in bioinorganic and bioinorganic systems elegantly demonstrate the symbiotic and synergistic interplay of covalent and non-covalent bonds, neither working correctly without assistance from the other. This presentation will discuss minimalist synthetic models of biological electron transfer that exploit (i) cascade proton transfer, or (ii) hydrogen bonds in the secondary coordination sphere to regulate the thermodynamics and dynamics of electron transfer.

Symposium : **KCS5-2**

[Mini Symposium on Lab Safety] Understanding of The Severe Accident Punishment Act

Room 302 WED 15:00

Chair: Ik-Mo Lee (Inha University)

"Effective countermeasures of companies/institutions according to the enforcement of the Serious Accidents Punishment Act": Focusing on field experience

HyukSeung Yang

Korea Risk Management Solutions, Korea

Although the Serious Accidents Punishment Act was enforced on January 27, 2022, the subject and scope of application of the Act's obligation to secure safety and health has not been specified in industrial sites, causing confusion. Large companies and institutions with financial capacity are trying to respond to the responsibilities and roles of employers and chief executives through legal advice from law firms, but most industrial sites are not presented with clear standards for the scope of safety-related laws. Large companies and institutions have mostly established safety and health management systems for their obligations to secure safety and health, but relatively small companies and institutions need a lot of time to build their own systems and systematically implement safety and health management. In addition, as companies and institutions focus only on complying with safety and health laws, systematic management is rarely carried out, and by entrusting safety and health management to external safety and health agencies, it is overlooked in terms of securing safety and health. The purpose of the Act is to strengthen the obligation to secure safety and health to employers and chief executives to prevent industrial accidents by discovering harmful and risk factors existing in the workplace in advance. Therefore, in order to secure safety and health of companies and institutions, it is necessary to make more efforts to secure safety and health by the workplace itself rather than relying on external institutions.

Symposium : **KCS6-1**

[BKCS Symposium] Where to go: The First Leap towards a Better Future of BKCS!

Room 401 THU 15:40

Chair: Nak Cheon Jeong (DGIST)

Current State of the BKCS and Future Strategy

Nak Cheon Jeong

Department of Physics & Chemistry, DGIST, Korea

The Bulletin of the Korean Chemical Society (BKCS) is the Korean Chemical Society (KCS) 's flagship research journal, founded in 1980 to reach the chemical community worldwide. The BKCS, where all papers are published on Wiley Online Library (WOL) with the support of the KCS, is a strictly peer-reviewed journal and welcomes Communications, Articles, Personal Accounts, and Reviews written in English. The scope of the BKCS covers all major areas of chemistry: analytical chemistry, electrochemistry, industrial chemistry, inorganic chemistry, life-science chemistry, macromolecular chemistry, organic synthesis, non-synthetic organic chemistry, physical chemistry, and materials chemistry. In this talk, BKCS's current editorial board and the history, current state, and future strategy of the BKCS will be presented.

Symposium : **KCS6-2**

[BKCS Symposium] Where to go: The First Leap towards a Better Future of BKCS!

Room 401 THU 15:50

Chair: Nak Cheon Jeong (DGIST)

Induced Transformation toward Itself via Disproportionation

Dongwon Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of of $Hg(OTf)_2$ with naphthalene-2,6-diyldipicolinate (L) in a mixture of 3-pentanone and dichloromethane produced the unusual catenated matallacycle of $[Hg_4(OTf)_4L_2]$ via straightforward formation of reduced Hg_2^{2+} as a skeletal synthon whereas the reaction in a mixture of acetonitrile and chloroform gave rise to metallacyles of $[Hg_2(OTf)_4L_2]$ via simple cyclization. The most important feature is that he successive addition of $[Hg_2(OTf)_4L_2]$ into $[Hg_4(OTf)_4L_2]$ in acetonitrile converged a product of $[Hg_2(OTf)_4L_2]$ quantitatively.

Symposium : **KCS6-3**

[BKCS Symposium] Where to go: The First Leap towards a Better Future of BKCS!

Room 401 THU 16:10

Chair: Sungjin Park (Inha University)

Porphyrinoids, a unique platform for exploring excited-state aromaticity

Dongho Kim

Department of Chemistry, Yonsei University, Korea

Recently, Baird (anti)aromaticity is referred to as a description of the excited-state (anti)aromaticity. With a term of Baird’s rule, recent studies have intensively verified that the Hückel aromatic [4n+2]π (or antiaromatic [4n]π) molecules in the ground state is reversed to Baird aromatic [4n]π (or Baird antiaromatic [4n+2]π) ones in the excited states. [1,2] As the Hückel (anti)aromaticity has great influence on the molecular properties and reaction mechanisms, the Baird (anti)aromaticity has been expected to act as a dominant factor in governing excited-state properties and processes, which brought intensive scientific investigations for the verification of the concept of reversed aromaticity in the excited states, the aromaticity reversal. [3,4] In this scientific endeavors, porphyrinoids recently play a leading role in the demonstration of the aromaticity reversal in the excited states and its conceptual development. [5] The distinct structural and electronics nature of porphyrinoids depending on their (anti)aromaticity allows for a direct observation of excited-state aromaticity reversal, Baird’s rule. Furthermore, the explicit experimental demonstration with porphyrinoids has contributed greatly to its conceptual development and application into novel functional organic materials. Based on the significant role of porphyrinoids in the field of excited-state aromaticity, this review provides an overview of experimental verification of the reversal concept of excited-state aromaticity by porphyrinoids and recent progress with its conceptual application to novel functional molecules.References[1] Sung, Y. M.; Yoon, M.-C.; Lim, J. M.; Rath, H.; Naoda, K.; Osuka, A.; Kim, D. Nat. Chem. 2015, 7 (5), 418–422.[2] Oh, J.; Sung, Y. M.; Hong, Y.; Kim, D. Acc. Chem. Res. 2018, 51 (6), 1349–1358.[3] Kim, J.; Oh, J.; Park, S.; Zafra, J. L.; DeFrancisco, J. R.; Casanova, D.; Lim, M.; Tovar, J. D.; Casado, J.; Kim, D. Nat. Commun. 2019, 10 (1), 4983. [4] Ueda, M.; Jorner, K.; Sung, Y. M.; Mori, T.; Xiao, Q.; Kim, D.; Ottosson, H.; Aida, T.; Itoh, Y. Nat. Commun. 2017, 8 (1), 346. [5] Kim, J.; Oh, J.; Osuka, A.; Kim, D. Chem. Soc. Rev. 2022, 51 (1), 268–292.

Symposium : **KCS6-4**
[BKCS Symposium] Where to go: The First Leap towards a Better Future of BKCS!
Room 401 THU 16:30
Chair: Sungjin Park (Inha University)

Perovskite Solar Cell: A Game Changer in Photovoltaics

Nam-Gyu Park

School of Chemical Engineering, Sungkyunkwan University, Korea

Since the ground-breaking report of the 9.7% efficient and 500 h-stable solid-state perovskite solar cell (PSC) in 2012 based on methylammonium lead iodide, perovskite photovoltaics have been surged swiftly due to high power conversion efficiency (PCE) obtainable via facile fabrication procedure. As a result, a PCE of 25.7% was recorded in 2022. According to Web of Science, number of publications on PSCs increases exponentially since 2012, leading to the accumulated publications of more than 26,000 as of February, 2022. PSC is thus regarded as a game changer in photovoltaics because of low-cost and high efficiency surpassing the conventional high efficiency thin film technologies. High photovoltaic performance was realized by compositional engineering, device architecture and fabrication methodologies for the past 10 years. Toward theoretical efficiency over 30% and entering market, further studies on recombination and scalable technologies are required for next 10 years. In this talk, scientific and technological approaches for high efficiency and large-area coating are discussed. For high efficiency, not only perovskite materials and coatings but also interfacial engineering via additive and post-treatment is of importance. For up-scaling PSCs, precursor formulation and coating methods are critical in determining photovoltaic performance. Stability issue will be also discussed and methodologies to improve stability are suggested.

Symposium : **KCS6-5**

[BKCS Symposium] Where to go: The First Leap towards a Better Future of BKCS!

Room 401 THU 16:50

Chair: Sunwoo Lee (Chonnam National University)

Metal-Free Amination Reactions: Mechanistic Strategy and Synthetic Applications

Sukbok Chang

Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea

Synthesis of heteroarylamines has been an important topic in organic chemistry due to their importance in small molecule discovery. In particular, 2-aminopyrimidines represent a highly privileged structural motif that is prevalent in bioactive molecules. While they are conventionally accessed through substitution of pre-functionalized substrates, a general strategy to introduce the pyrimidine C2–N bonds via direct functionalization is elusive. In this context, we have developed a synthetic platform for site-selective heteroaryl C–H functionalization that affords heteroaryl iminium salt intermediates, which can be transformed into various amine products in situ. Mechanism-based reagent design allowed for the C2-selective amination of pyrimidines and C4-amination of pyridines, opening the new scope of site-selective heteroaryl C–H functionalization. Our method is compatible with a broad range of heteroarenes with sensitive functional groups, and can access complex heteroarylamines in high selectivity.

Symposium : **KCS6-6**
[BKCS Symposium] Where to go: The First Leap towards a Better Future of BKCS!
Room 401 THU 17:10
Chair: Sunwoo Lee (Chonnam National University)

Recent Progress on Activatable Photosensitizers and Fluorescent Probes

Juyoung Yoon

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Switchable phototheranostic nanomaterials are of particular interest for specific biosensing, high-quality imaging, and targeted therapy in the field of precision nanomedicine. Here, we develop a “one-for-all” nanomaterial (NanoPcTBs) that self-assembles from flexible and versatile phthalocyanine building blocks. Fluorescence and reactive oxygen species (ROS) generation could be triggered depending on a targeted, protein-induced, partial disassembly mechanism, which creates opportunities for low-background fluorescence imaging and activatable photodynamic therapy (PDT). On the other hand, the in vivo specific binding between albumin and PcS, arising from the disassembly of injected NanoPcS, was recently confirmed using an inducible transgenic mouse system. In a recent investigation, we devised a novel molecular design approach to create heavy-atom-free photosensitizers for thionapthalimides and BODIPYs. The thionaphthalimides display dramatically enhanced quantum yields for photosensitized singlet oxygen formation. Relying on abnormal alkaline phosphatase (ALP) activity, DQM-ALP was successfully used to differentiate between tumors tissues and normal tissues in nude BABL/c mice bearing HepG-2 and HeLa xenograft tumors. In addition, a near-infrared two-photon fluorescent probe was developed to not only specially image carboxylesterase (CE) activity in vivo and in situ but also target orthotopic liver tumor after systemic administration.

Award Lecture in Division : **POLY1-5**

Recent Researches on Polymer Chemistry from the Perspective of Industrialization

Samda Hall THU 17:20

Chair: Jeyoung Park (KRICT)

Polymers from Functionalized Norbornenes

Jeewoo Lim

Department of Chemistry, Kyung Hee University, Korea

Norbornenes are rigid bicyclic structures possessing high ring strain energy, the release of which is the driving force for ring-opening metathesis polymerization (ROMP). The structure of norbornenes also allows for an interesting annulation reaction with functionalized arenes, which is utilized in the catalytic arene-norbornene annulation (CANAL) polymerization to prepare ladder polymers. We herein report our recent progress on the utilization of various functionalized norbornenes as monomers in CANAL polymerization and dispersion ROMP. A bis(norbornene) bearing heterocyclic core structure has been utilized to prepare ladder polymers through CANAL polymerization. Norbornenes with high fluorine contents of over 50 wt% have been polymerized to yield fluorinated polynorbornenes, the low solubilities of which was addressed through the development of fluorous dispersion ROMP (FD-ROMP), which could be expanded to metal-free versions of the polymerization. The developments allowed for the achievement of ladder polymers containing heterocycles in the main chain and a dispersion ROMP capable of producing fluoropolymers in multigram scales.

Symposium : **POLY1-1**

Recent Researches on Polymer Chemistry from the Perspective of Industrialization

Samda Hall THU 15:40

Chair: Jeyoung Park (KRICT)

Trends of Surface-Finishing Technology for Interior and Exterior Plastic Parts in Automotive

Hotak Jeon

Interior System Plastic Materials Development Team, HYUNDAI MOTOR COMPANY, Korea

One of the most basic requirements for automotive interior & exterior plastic parts is perceived quality. Perceived quality such as sight (color / pattern / mood lighting), hearing (noise reduction), touch (soft feeling), and smell (indoor smell / VOCs) are very important factors that can impress customers. The surface-finishing technology for plastic parts is a surface decoration technology for improving perceived quality, luxury and durability, and various surface-finishing technologies such as painting, plating, film, and real materials are applied to automotive plastic parts. In addition, many surface-finishing technologies have been developed for each vehicle class to differentiate them from competitors.

Electrification and sharing of vehicles are major trends in the automotive market. Since Electric vehicle is an eco-friendly vehicle that can improve environmental problems such as greenhouse gas reduction, it is necessary to develop interior materials suitable for the image of an eco-friendly vehicle. Also, customer needs for vehicle hygiene and health care are gradually increasing due to the COVID -19 issue. In this presentation, we would like to present the direction of developing surface-finishing technology for plastic parts in future mobility.

Symposium : **POLY1-2**

Recent Researches on Polymer Chemistry from the Perspective of Industrialization

Samda Hall THU 16:05

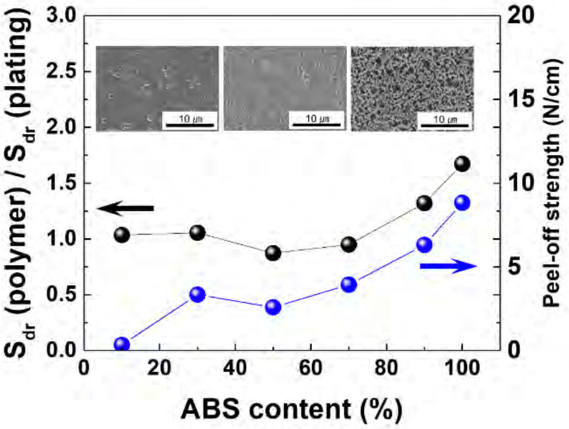
Chair: Jeyoung Park (KRICT)

Morphology formation of PC/ABS blend and its application to the electroplating

Jaesik Seo

Interior System Plastic Materials Development Team, Hyundai Motor Company, Korea

Polycarbonate/acrylonitrile-butadiene-styrene (PC/ABS) is one of the most versatile polymer blends in automotive industry. Accordingly, it has been widely used irrespective of interior/exterior parts. Twin screw-extruded PC/ABS exhibited morphological phase transition from needle-like co-continuous to sea-island structure when ABS content exceeded 50 wt%. The rheological yield stress of PC/ABS blend recorded the highest value at the blend ratio of 3:7, which indicates that the strongest internal structure was generated between two polymers. The presence of ABS in the PC matrix induces significant change on fracture behavior of PC, transitioning from brittle to ductile nature. This phenomenon brings about abrupt improvement in impact strength. We applied the morphological characteristics of PC/ABS blend to the electroplating process and investigated quantitative relation between interfacial morphology and adhesion strength of metal-plated polymer substrate. Physically interlocked interfacial adhesion strength could be predicted by using newly proposed Sdr parameter, developed surface area relative to the plane surface.


S_{dr} (polymer) / S_{dr} (plating)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
20
40
60
80
100
ABS content (%)
Peel-off strength (N/cm)
20
15
10
5
0
10 μm
10 μm
10 μm

Symposium : **POLY1-3**
Recent Researches on Polymer Chemistry from the Perspective of Industrialization
Samda Hall THU 16:30
Chair: Jeyoung Park (KRICT)

Flexible Chemical Sensor Film

Hoyoul Kong*, Ka Yeon Ryu

Department of Chemistry, Gyeongsang National University, Korea

Chemical sensors for trace detection of hazardous chemicals have been investigated for environmental remediation, public safety, military and homeland defense applications because of terrorist threats. Organic field-effect transistor (OFET) and Resistor based film sensors have been proposed and investigated, possess advantages of easy tuning of chemical and physical properties, low-cost processing, and mechanical flexibility, and as sensors they offer fast readout on analyte exposure from simple probes and meters. In this talk, I will introduce various sensor materials and chemical film sensor applications for detection of chemical analytes.


Flexible Display


Flexible Sensor

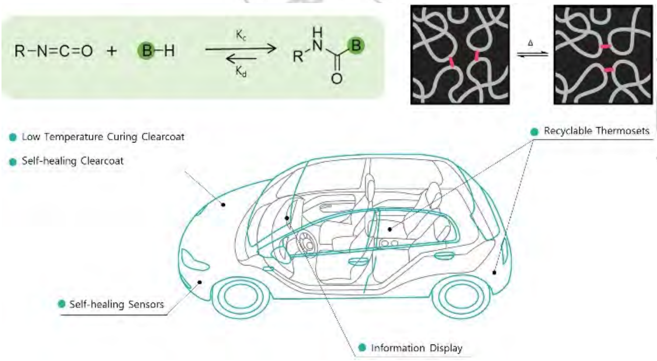
Symposium : **POLY1-4**
Recent Researches on Polymer Chemistry from the Perspective of Industrialization
Samda Hall THU 16:55
Chair: Jeyoung Park (KRICT)

Design and Applications of Dynamic Covalent Bonds and Polymer Networks for Next Generation Automotive Parts

Jin chul Kim

정밀화학융합기술연구센터, Korea Research Institute of Chemical Technology, Korea

Recently, dynamic covalent bonds have been received much attention from both academia and industry due to their potential applications as thermal latent catalysts and curing agents, self-healing and shape memory polymers, and recyclable thermoset elastomers. In the first part of the presentation, we report materials design and quantitative analysis techniques of diverse dynamic polymer networks based on the thermally reversible dynamic bonds such as Diel-Alder adduct, hindered urea bond, and carbamate bond. In the second part, industrial applications of dynamic covalent bond in low temperature curing automotive clearcoat, recyclable polyurethane thermosets, and self-healing coatings will be introduced.



Symposium : **POLY2-1**

Symposium by Mid-career Polymer Chemists

Samda Hall FRI 09:00

Chair: Myungeun Seo (KAIST)

Controlling molecular interactions for applications of graphene and boron nitride nanotubes

Seokhoon Ahn

Institute of Advanced Composite Materials, Korea Institute of Science and Technology, Korea

Understanding and controlling interface structures between organics and nanomaterials such as graphene and boron nitride nanotubes (BNNTs) play a critical role to make commercialization of nanomaterials successful. For example, although graphene has been attracted for a number of applications such as gas barrier films, transistors, and electrodes, the commercialization of graphene has not been successful due to structural defects and high sensitivity to environmental conditions. These problems could be solved by introducing ordered organic molecules to graphene surface through van der Waals interactions. The scanning tunneling microscopy (STM) study reveals that alkane molecules could be close-packed on graphene, resulting in blocking outside dopants and graphene defects. For BNNTs, the bottle neck of BNNTs commercialization is purification due to impurites such as h-BN which has similar chemical properties with BNNTs. This bottle neck could be solved by functionalization of BNNTs with polymers which could do dipole-dipole interaction with BNNTs.

Symposium : **POLY2-2**

Symposium by Mid-career Polymer Chemists

Samda Hall FRI 09:25

Chair: Myungeun Seo (KAIST)

Influence of Molecular Weight on Molecular Doping Efficiency and Thermoelectric Properties

BongSoo Kim

Department of Chemistry, UNIST, Korea

We studied the effect of molecular weight of a series of conjugated polymers (CPs) on the doping efficiency, electrical conductivity, and related thermoelectric properties of doped CPs. Low (L), medium (M), and high (H) molecular weight of PDFD-T polymers, based on difluorobenzothiadiazole and dithienosilole moieties, were synthesized and denoted as PDFD-T(L), PDFD-T(M), and PDFD-T(H), respectively. Furthermore, to compare the effects of different donor moieties, donor units of PDFD-T(L) were structurally modified from thiophene to thienothiophene (TT) and dithienothiophene (DTT), denoted as PDFD-TT(L) and PDFD-DTT(L), respectively. After doping the CPs with FeCl3, doped(d) PDFD-T(H) exhibited an electrical conductivity of over 400 Scm-1, which is significantly higher than those of d-PDFD-T(L), d-PDFD-T(M), d-PDFD-TT(L), and d-PDFD-DTT(L). Through various characterizations, we demonstrated that the molecular weight of CPs has a strong influence on the degree of doping and directly affects the crystallinity of the CP films and the formation of charge transporting pathways in doped films. CPs with a high molecular weight have a high carrier mobility while maintaining their original morphology and high carrier mobility even after doping. The highest power factor of >100 μWm-1K-2 was achieved through organic thermoelectric devices fabricated using PDFD-T(H). Therefore, we suggest that optimizing the molecular weight of CPs is an essential strategy for maximal power generation from their doped CP films. Overall, our work demonstrates that controlling the molecular weight of CPs can provide a key solution to minimize the crystallinity degradation of doped CPs, ultimately optimizing the doping efficiency, electrical conductivity, and thermoelectric properties.

Symposium : **POLY2-3**

Symposium by Mid-career Polymer Chemists

Samda Hall FRI 10:00

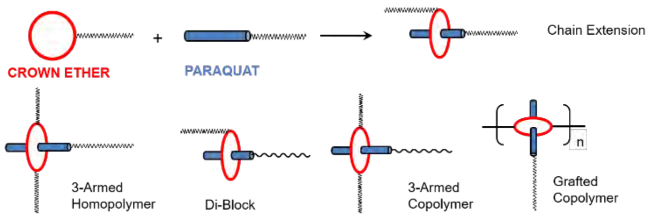
Chair: Myungeun Seo (KAIST)

Various polymer topologies from self-assembling host and guest building blocks

Minjae Lee

Department of Chemistry, Kunsan National University, Korea

Host-guest systems have been utilized to construct desired supramolecular architectures by their self-assembling behaviors. Pseudorotaxane formation from crown ethers and viologens is one of the representative host and guest combinations in supramolecular science. In this study, combinations of well-designed host and guest building blocks formed pseudorotaxane units and they constructed various polymer topologies; chain extended linear polymers, linear dibock copolymers, graft copolymers, and hyperbranched polymers. These physically interlocked pseudorotaxanes and rotaxanes and they could be easily dissociated to go back to each building block by high polar solvent, such as dimethyl sulfoxide. Two strategies were used for the supramolecular polymers. The first method was from the combinations of “polymer building blocks”, which were prepared by controlled radical polymerization. This reactions gave a host or a guest end (or center) unit on each polymer chain. The existence of the crown or the viologen functionality was confirmed by high resolution mass spectrometry with soft ionization techniques. Desired polymer topologies were realized by just dissolution of the well-designed host and guest polymer building blocks. The second method used “post polymerization”, which gave A_2B_2 four-armed supramolecular block copolymers from the pseudorotaxane macro-initiator. Detail characterizations and evidences for the various polymer formations will be presented.



Symposium : **POLY2-4**

Symposium by Mid-career Polymer Chemists

Samda Hall FRI 10:25

Chair: Myungeun Seo (KAIST)

Orienting and aligning molecules in supramolecular polymeric cryopreservation nanoagents

Eunji Lee

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea

Supramolecular polymeric assembly of peptides has been blessed to hold the well-defined nanostructures by incorporation of amino acid building blocks to realize the customized functions, that can be utilized as a scaffold in bioactive catalyst, drug delivery, regenerative medicine, and tissue engineering. The structural diversity and stability could be acquired by control of secondary structure and non-covalent interactions. Cryopreservation has evolved as an important technology required for biotechnological, pharmaceutical, biochemical or food industries for the storage purpose of protein drugs, cells, tissues and food, and ice slurries. Antifreeze protein (AFP) has been received attention with its potential as a cryopreservation agent by its ability to prevent the organisms from freezing in the subzero environment through antifreeze activity such as ice recrystallization inhibition or thermal hysteresis effect. However, it is struggling to apply the natural AFP in practical industries as a cryopreservation agent because of their irreversible denaturation and the difficulty in extraction from nature. Here, I will introduce the natural AFP mimetic short peptides showing antifreeze activity. Ice nucleation and growth was controlled by the spacing of molecules matching the ice lattice and the alignment and orientation of molecules affecting the interaction with ice. The customized agents by considering supramolecular chemistry increase cell-cryopreservation activity and reduce cell damage. This research might provide a useful strategy to fabricate the cryopreservation agent through the supramolecular nanomaterials and to figure out the mechanism of antifreeze protein binding to ice.

Symposium : **POLY3-1**
Recent Trends in Early-career Polymer Chemists
Samda Hall FRI 14:30
Chair: Byungjin Koo (Dankook University)

Functional Polymer Wrapped Single-Walled Carbon Nanotubes for Chemiresistive Sensors

Seon-Jin Choi

Division of Materials Science and Engineering, Hanyang University, Korea

Carbon nanotubes are widely employed as an electrical transducer for application in chemiresistive sensors considering their high electrical conductivity. In addition, the large surface area of carbon nanotubes is advantageous for the sensitive detection of analytes with high response. However, the non-selective property of pristine carbon nanotubes is a critical issue for the recognition of target analytes. In this regard, various selector molecules were decorated on the surface of carbon nanotubes to increase the selective property.In this presentation, I will introduce the recent progress of non-covalently functionalized single-walled carbon nanotubes (SWCNTs) for applications in chemiresistive sensors.[1-4] Functional polymers were synthesized by decorating selector groups, which can have a chemical interaction with target analytes such as gas molecules and ionic species in solution. The chemiresistive sensing layer of SWCNTs was non-covalently functionalized by wrapping with functional polymers. As a result, real-time electrical transduction was achieved upon the injection of a chemical analyte with high sensitivity and selectivity. The chemiresistive sensor was integrated with a wireless sensing module for application in real-time wireless detection of analytes. The proposed SWCNT-based sensing platform with functional polymers can be applied in various fields such as environmental monitoring and healthcare.[1] S.J. Choi, B. Yoon, J.D. Ray, A. Netchaev, L.C. Moores, T.M. Swager, Chemiresistors for the Real-Time Wireless Detection of Anions, Adv Funct Mater, 30(2020).[2] S.J. Choi, B. Yoon, S.B. Lin, T.M. Swager, Functional Single-Walled Carbon Nanotubes for Anion Sensing, ACS Appl Mater Inter, 12(2020) 28375-82.[3] B. Yoon, S.J. Choi, Selective acetate recognition and sensing using SWCNTs functionalized with croconamides, Sensor Actuat B-Chem, 346(2021).[4] B. Yoon, S.J. Choi, T.M. Swager, G.F. Walsh, Flexible Chemiresistive Cyclohexanone Sensors Based on Single-Walled Carbon Nanotube-Polymer Composites, ACS Sensors, 6(2021) 3056-62.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **POLY3-2**
Recent Trends in Early-career Polymer Chemists
Samda Hall FRI 14:55
Chair: Byungjin Koo (Dankook University)

Vinyl-Addition Copolymerization of Norbornene and Its Ester Derivative toward Cyclic Olefin Copolymer with Randomly Distributed Polar Groups

Chang-Geun Chae

Advanced Functional Polymers Research Center, Korea Research Institute of Chemical Technology, Korea

Since development of transition metal catalysts for coordination-insertion polymerization of olefins, their utilization have been extended to create cyclic olefin polymers with novel material properties. The most popular model, vinyl-type polynorbornene, has drawn interest as a promising optical material owing to its excellent properties, such as high thermal stability, high glass transition temperature, and high optical transparency. However, some unfavorable properties (poor solubility, high brittleness, and low surface energy) attributed mostly to its non-polar structure have highly limited its application. To solve this issue, the copolymerization of norbornene and its polar derivatives has been studied by many polymer chemists. Although several nickel and palladium complexes have been suggested as effective copolymerization catalysts, the random polar group distribution has remain a necessary challenge to achieve not only homogeneous polymer structure but also precise control of polar group introduction. We developed several nickel complexes that are effective for the synthesis of random copolymer of norbornene and its polar ester derivative. In this presentation, we show a principle of catalyst design to minimize the monomer selectivity, and describe the effects of controlled ester group incorporation on various copolymer properties.

Symposium : **POLY3-3**

Recent Trends in Early-career Polymer Chemists

Samda Hall FRI 15:20

Chair: Byungjin Koo (Dankook University)

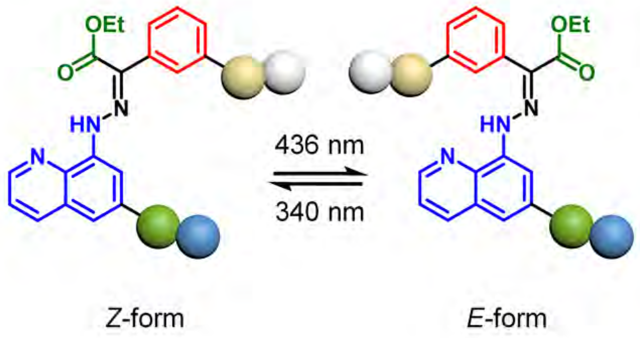
Hydrazone Photoswitches for Structural Modulation of Short Peptides

Sunbum Kwon

Department of Chemistry, Chung-Ang University, Korea

Molecules that undergo light-driven structural transformations constitute the core components in photoswitchable molecular systems and materials. Among various families of photoswitches, photochromic hydrazones have recently emerged as a novel class of photoswitches with superb properties, such as high photochemical conversion, spectral tunability, thermal stability, and fatigue resistance. Hydrazone photoswitches have been adopted in various adaptive materials at different length scales, however, their utilization for modulating biomolecules still has not been explored. Herein, we present new hydrazone switches that can photomodulate the structures of short peptides. Systematic investigation on a set of hydrazone derivatives revealed that installation of the amide group does not significantly alter the photoswitching behaviors. Importantly, a hydrazone switch comprising an upper phenyl ring and a lower quinolinyl ring was effective for structural control of peptides. We anticipate that this work, as a new milestone in the research of hydrazone switches, will open a new avenue for structural and functional control of biomolecules.

Light-driven structural control of peptides



Symposium : **POLY3-4**

Recent Trends in Early-career Polymer Chemists

Samda Hall FRI 15:45

Chair: Byungjin Koo (Dankook University)

Molecular Design Strategies for Developing Polymeric Hole Transport Materials in Perovskite Photovoltaics

Jea Woong Jo

Department of Energy and Materials Engineering, Dongguk University, Korea

Recently, perovskites have garnered worldwide research interest as promising candidate materials for next-generation photovoltaic devices owing to their unique optoelectronic properties. Typical perovskite photovoltaics (PPVs) are fabricated with a sandwich configuration comprising a parallel cathode and anode upon which an electron-transporting material and a hole-transporting material (HTM) are deposited, respectively. To realize highly efficient and stable PPVs, the interface layer materials should satisfy several requirements: 1) Suitable energy levels that minimize potential energy loss at the perovskite/electrode interface and increase charge selectivity at the corresponding electrodes; 2) high hole or electron mobility for efficient charge transport and charge collection; and 3) high resistance to humidity and photodegradation for long-term device stability. In this presentation, we will present a new class of polymeric HTMs for flexible p-i-n PPVs by introducing conjugated polyelectrolyte structure. Then, the strategies for improving the interaction between perovskite and polymeric HTMs for high performance n-i-p PPVs will be discussed.

Symposium : **INOR1-1**

A New Horizon in Inorganic Chemistry

Tamna Hall B THU 15:40

Chair: Eunsung Lee (POSTECH)

Bio-AFM: Ultrasensitive Tool for Liquid Biopsy and Bioanalysis

Joon Won Park

Department of Chemistry, Pohang University of Science and Technology, Korea

In 2005, we applied a new surface modification approach to coat AFM probes, and observed that the coating guarantees truly 1:1 interaction between a DNA on the probe and a complementary DNA on a solid substrate. Such coating approach enhanced accuracy of the measurement at the single molecule level. Through a long academic journey to year of 2021, we were able to demonstrate that AFM is capable of detect very low copy number of mutated genes in solution without amplfication or labeling. We also showed that the tool paves a new avene for liquid biopsy, an attractive approach for early cancer detection. In the seminar, I will introduce a core story of the journey and a plan for the future. (end)

Symposium : **INOR1-2**

A New Horizon in Inorganic Chemistry

Tamna Hall B THU 16:10

Chair: Eunsung Lee (POSTECH)

Sustainable Polyolefin Developments Toward a Better Future

Choong Hoon Lee

Senior Research Fellow, Polyolefin Department Leader, Korea

As global climate crisis and resource depletion issues have recently emerged, the ESG management of many companies have been attended increasingly. In line with this global trend, many leading companies including the governments are changing the business environment along with social contribution and transparent management. In this lecture, I would like to talk about how LG Chem manages important issues such as renewable resources, biomaterials and recycled products in the petrochemical industry. In particular, polyolefin products which account for the largest proportion in the synthetic polymer industry are mainly used for packaging and construction materials, but we should solve these problems through recycling of packaging materials or weight reduction of materials due to global environment issue. In addition, LG Chem plans to contribute to carbon neutrality through the development of energy materials such as solar power in the polyolefin field. We would like to the direction of the development of polyolefin materials with a focus on related contents.

Symposium : **INOR1-3**

A New Horizon in Inorganic Chemistry

Tamna Hall B THU 16:40

Chair: Eunsung Lee (POSTECH)

Energy Storage in Chemical Bonds for Carbon Neutrality

Chang Won Yoon

Chemical Engineering, Pohang University of Science and Technology, Korea

To address the current energy and environmental issues, an increase in renewable energy production is necessary . Due to the intermittent and unpredictable nature of renewable energy production, however, the renewable energy must be stored and re-produced on demand. Hydrogen is considered as a clean renewable energy carrier because of its high gravimetric energy storage density of ca. 33.3 kWh·kg-1. But, the low volumetric energy density of gaseous hydrogen (2.97 Wh·L-1@273 K & 1 atm) limited its use particularly for high capacity and long distance hydrogen transportation. In the context, a safe and economically viable hydrogen storage system that enables to transport mass quantities of hydrogen in a chemical form has attracted significant attention. Promising inorganic and organic based materials for this purpose include liquid organic hydrogen carriers (LOHCs) and ammonia (NH3) which allow hydrogen to be stored and released reversibly through chemical reactions. In the presentation, recent trends for chemical hydrogen storage technology utilizing LOHC and NH3 will be introduced.

Symposium : **INOR1-4**

A New Horizon in Inorganic Chemistry

Tamna Hall B THU 17:00

Chair: Eunsung Lee (POSTECH)

A platform to enhance quantitative single-molecule technology

Yoonhee Lee

Division of Electronics and Information System, Daegu Gyeongbuk Institute of Science & Technology, Korea

As one of the leaders in the field of single-molecule technologies, Prof. Joon Won Park has achieved exciting developments in fundamental single-molecule research and real-world applications. In this talk, I am highlighting a selection of Prof. Park’s works on the detection and quantification of single DNA molecules. We developed a novel single-molecule detection platform based on capturing target DNAs on the chemically engineered surface and analyzing individual DNAs at the nanoscale with atomic force microscopy (AFM). This technology provides single-molecule sensitivity without amplification nor labeling and has been demonstrated with various target DNAs showing promising results as a potent clinical diagnosis tool. The research experiences with Prof. Park and his brilliant guidance have shaped my current research interests, which are focusing on nanointerface platforms for portable single-molecule technology and personalized diagnostics.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **INOR1-5**

A New Horizon in Inorganic Chemistry

Tamna Hall B THU 17:20

Chair: Eunsung Lee (POSTECH)

Molecular swarm agents for massively parallel inspection and reconstruction of molecular landscapes

Sungwook Woo

Department of Chemistry, Pohang University of Science and Technology, Korea

Current methods of studying molecular systems are often limited in throughput, because they either treat all molecules equally (as in ensemble measurements) or examine one molecule at a time (as in single-molecule measurements). In this talk, an approach based on molecular swarm agents for surveying molecular landscapes will be presented. Molecular swarm agents are DNA-based motors that can copy information from targets and generate records that reflect the trajectory. A swarm of agents can roam around and record spatial organizations of molecular systems and their conditional changes in a massively parallel manner, with each agent reporting information on local arrangements and collectively allowing us to reconstruct the global map. Data will be presented demonstrating the basic mechanisms and a few model systems where the agents were used to count the number of subunits in molecular complexes or to detect the state changes in molecular arrangements. This technology will enable new capabilities in fundamental molecular sciences by providing an unprecedented tool for parallel and multiplexed examination of molecular systems.

Symposium : **INOR2-1**

Recent Trends in Inorganic Chemistry

Tamna Hall B FRI 09:00

Chair: Hyo Jae Yoon (Korea University)

Induced Formation of Specific Metal-Organic Frameworks (MOFs); Towards the Ideal MOFs

Moonhyun Oh

Department of Chemistry, Yonsei University, Korea

Metal-organic frameworks (MOFs) and porous coordination polymers (CPs) have attracted many attentions not only due to their various structural topologies and chemical tunabilities but also their many useful properties and applications, such as gas storage, gas separation, catalysis, sensing, and recognition. Currently, various ongoing research have been devoted to the development of more functional or useful MOFs with enhanced property and applicability. The conjugation of MOF materials with other materials, such as silica, polystyrene, magnetic particle, and metal particle, is a noble strategy for producing MOF-based hybrid materials. Not only the conjugation of MOFs with other materials but also the controlled conjugation of MOF with different types of MOFs to form the complicated MOFs containing more than two types of MOFs is a noteworthy approach in the MOF development; this is because the management of the composition and structure of MOFs is essential for fine tuning their properties and applicability. These complicated or hybrid MOF materials with precise hetero-compositions or hetero-structures will provide great opportunities to overcome MOF's inherent weak points or to obtain user's desirable properties. Here I present the understanding on the precise MOF-on-MOF growth process and so the controlled construction of complicated MOFs based upon the MOF-on-MOF growth. The work described here will provide a way to access a variety of multi-compositional or multi-structural MOF-based materials, something that should facilitate their eventual use in practical applications.

Symposium : **INOR2-2**

Recent Trends in Inorganic Chemistry

Tamna Hall B FRI 09:30

Chair: Hyo Jae Yoon (Korea University)

Mechanical Gating of Canopied Cavitand: Leverage, Transmission, and Cooperativity

Dongwhan Lee

Department of Chemistry, Seoul National University, Korea

Container molecules can be designed to recruit multiple guests into a confined space to enhance host-guest interactions or to accelerate chemical reactions. For such schemes to work, the initial complexation should cooperatively promote subsequent binding events. We built a previously unknown shape-adaptive molecular basket that opens and closes its canopies to bind two guest molecules. The highly cooperative nature of this supramolecular interaction was hinted by unusual binding isotherms, but could not be fully resolved by standard numerical fitting protocols. A new graphical representation was thus devised that is based solely on the first principles of chemical equilibrium to interpret the spectroscopic signatures of cooperativity. This presentation will discuss the underlying molecular mechanism of this intriguing process.

Symposium : **INOR2-3**
Recent Trends in Inorganic Chemistry
Tamna Hall B FRI 10:00
Chair: Hyo Jae Yoon (Korea University)

Systematic Discovery of Materials with Noncentrosymmetric Structures

Kang Min Ok

Department of Chemistry, Sogang University, Korea

Functional inorganic materials crystallizing in noncentrosymmetric (NCS) structures have been attracting massive attentions owing to their structure-related various characteristics such as second-harmonic generation (SHG), piezoelectric, pyroelectric, ferroelectric, and multiferroic properties. A range of useful applications such as medical lasers, telecommunications, lithography, detectors, energy harvesting, and data storage are expected from the materials with macroscopic NCS structures. Thus, improving the possibility of macroscopic NCS structures for synthetic solid-state materials is an ongoing challenge. One of the successful approaches is considered to introduce so-called NCS chromophores such as polyhedra with cations susceptible to second-order Jahn-Teller distortions, highly polarizable metal cations, and π-conjugated asymmetric anions with trigonal planar geometry. Unfortunately, however, the major reaction products still tend to crystallize in centrosymmetric structures possibility attributed to nature’s preference on symmetry. In this presentation, a few key factors influencing the framework structures as well as macroscopic centricity are suggested through careful structural examinations on recently reported materials containing asymmetric building units. Moreover, several systematic approaches toward the discovery of functional solid-state materials with NCS structures are proposed.

Symposium : **INOR2-4**

Recent Trends in Inorganic Chemistry

Tamna Hall B FRI 10:30

Chair: Hyo Jae Yoon (Korea University)

Photopatterned DNA-linked nanoparticle films for programmable shape changes

So-Jung Park

Department of Chemistry and Nano Science, Ewha Womans University, Korea

The self-assembly of nanoscale building blocks into complex nanostructures with controlled structural anisotropy can open up new opportunities for realizing active nanomaterials exhibiting spatiotemporal structural transformations. Here, we adopt a combination of bottom-up DNA-directed self-assembly and top-down photothermal patterning to fabricate free-standing nanoparticle films with vertical and lateral heterogeneity. This approach involves the construction of multi-component plasmonic nanoparticle films by DNA-directed layer-by-layer (LbL) self-assembly, followed by on-demand lateral patterning by the direct photothermal writing method. The distinct plasmonic properties of nanospheres and nanorods constituting the multi-domain films enable photopatterning in a selective domain with precisely controlled vertical depths. The photopatterned films exhibit complex morphing actions instructed by the lateral and vertical patterns inscribed in the film as well as the information carried in DNA.

Symposium : **INOR3-1**

Carbon-neutral Research in Inorganic Chemistry

Tamna Hall B FRI 14:30

Chair: Junhyeok Seo (GIST)

Designing Electrode-Electrolyte Interfaces for Selective Carbon Dioxide Conversion

Youngkook Kwon

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

Efficient electrochemical conversion of CO2 to fuels or stock chemicals with high-energy density would be a major step forward in the introduction of a carbon neutral energy cycle. Especially, understanding the role of electrocatalysts, supports, and electrolytes that can efficiently reduce CO2 to fuels with high selectivity is a subject of significant interest. Copper is the only known catalyst for producing a reasonable quantity of hydrocarbons, which means that designing proper electrode-electrolyte interfaces would modulate the catalytic reactivity and product selectivity. One of the representative observations on copper catalyst-electrolyte interface is that the selection of alkali cations has direct influence on activity and product selectivity; increasing the size of mono-valent cations can increase the activity and selectivity toward C-C coupled products by modulating the interaction energy between adsorbates and electric fields at the interface. Copper catalyst with a specific atomic-scale gap accelerates the reaction kinetics and selectivity to C2+ products. In addition, C-C coupling can be maximized by designing interfaces between copper and metal oxides. Therefore, designing electrode-electrolyte interface offers efficient, yet cheap electrochemical CO2 reduction systems.

Symposium : **INOR3-2**

Carbon-neutral Research in Inorganic Chemistry

Tamna Hall B FRI 14:55

Chair: Junhyeok Seo (GIST)

Rational Design of Solid Adsorbents for Post-Combustion CO2 Capture via Temperature Swing

Minkee Choi

Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology, Korea

Amine-functionalized porous materials have been extensively investigated as promising adsorbents for post-combustion CO2 capture due to their chemisorption ability of low-concentration CO2 (ca. 15%) from a wet flue gas. However, earlier studies in academia have mainly focused on the improvement of CO2 uptake of the adsorbents and there have been rather limited studies on other important engineering aspects of adsorbents such as regenerability, long-term stability, cost, and scalability of material production. In the present work, I will disclose our recent progresses on the adsorbent development for post-combustion CO2 capture. Our group developed a cost-effective and scalable synthesis method for amine/silica composite adsorbents that can simultaneously show large CO2 working capacities as well as outstanding stability (e.g., hydrothermal stability, urea stability, oxidation stability) in a practically meaningful temperature swing adsorption (TSA) condition (adsorbent regeneration under 100% CO2 at 110–120 ˚C). In particular, it will be demonstrated that controlled modification of polyethyleneimine (PEI) with epoxide-derivatives can markedly reduce the heat of CO2 adsorption and facilitates CO2 desorption compared to unmodified PEI during the adsorbent regeneration. The modification also significantly increased long-term adsorbent stability over repeated TSA cycles due to remarkable suppression of CO_2-induced urea formation and oxidative amine degradations.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **INOR3-3**
Carbon-neutral Research in Inorganic Chemistry
Tamna Hall B FRI 15:20
Chair: Junhyeok Seo (GIST)

20 K H2 physisorption on metal-organic frameworks with enhanced dormancy compared to liquid hydrogen storage

Hyunchul Oh

Department of Energy Engineering, Gyeongsang National University, Korea

Liquid hydrogen (LH2) is the best way of transporting hydrogen in terms of volumetric energy density. These benefits translate into a significant reduction in hydrogen transportation and refueling station operations expenses. However, the phase transformation from liquid to gaseous hydrogen is accompanied by a considerable volume change, making long-term storage or transportation problematic. Any heat leakage of the LH2 vessel will result in boil-off and a strong pressure increase, which finally has to be released. These boil-off losses are a severe drawback for continental (long-distance) transportation through truck tube trailers having evaporative losses of about 3-15 % per day depending on the volume. Herein, low-temperature hydrogen storage by cryo-adsorption using crystalline porous adsorbents is proposed as an alternative to reduce boil-off losses and enhance dormancy during long continental transportation. The volumetric H2 uptake in MOFs at 20 K can be comparable to the LH2 due to the stronger van der Waals adsorbate-adsorbent interaction than between adsorbate-adsorbate, leading to a higher H2 density inside the pores. As a result, the higher H2 density sufficiently compensates for the skeleton volume of the adsorbent, resulting in a volumetric storage capacity comparable to that of LH2 tanks (~ 95 %). Depending on the textural properties of MOFs, maximum H2 desorption temperature of 45 K can be achieved, resulting in an extended dormancy time of the tank system. In addition, the observation of hindered rotational transition (J : 0→1) signal in neutron scattering analysis indicates that the H2 molecules are firmly attached and highly immobile on the adsorption sites. The hindered rotation by adsorption at 20 K on MOFs also suggests that the intermolecular separation is less than the bulk liquid phase. Considering the above, these results can be exploited to design MOFs and optimize cryo-adsorbent-based H2 transportation and storage.

Symposium : **INOR3-4**

Carbon-neutral Research in Inorganic Chemistry

Tamna Hall B FRI 15:45

Chair: Junhyeok Seo (GIST)

Photocatalytic difunctionalization of C=C bonds with CO2

Sukwon Hong

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

The synthesis of carboxylic acids through direct carboxylation using carbon dioxide (CO2) has received much attention, as the products are important in medicinal chemistry applications and the preparation of fine chemicals. Over the last decade, sustainable photoredox catalysis in mild reaction conditions has been extensively studied as an important strategy in direct carboxylation for C-C bond formation with CO2. In particular, the photocatalytic difunctionalization of unsaturated hydrocarbons using CO2 has attracted much attention as a useful method for high value-added carboxylic acid derivatives. By using this strategy, both a carboxylic acid and another functional group are incorporated into unsaturated hydrocarbons in a single procedure with high atom- and step-economic efficiency. The metal-free photoredox-catalyzed carbocarboxylation of various styrenes with carbon dioxide (CO2) and amines to give γ-aminobutyric ester derivatives has been developed (up to 91%, 36 examples). Furthermore, photoredox-catalyzed α-aminoalkylcarboxylation of aryl allenes with CO2 and N,N-dimethylanilines has been developed (26 examples, up to 96% yield). In the case of electron-deficient allenes, good regioselectivity was observed (up to 94:6), exclusively generating kinetic products over thermodynamic products.

Symposium : **INOR3-5**

Carbon-neutral Research in Inorganic Chemistry

Tamna Hall B FRI 16:10

Chair: Junhyeok Seo (GIST)

Formic acid derivative production technology having both economic feasibility and the possibility of reducing greenhouse gas emissions

Sungho Yoon

Department of Chemistry, Chung-Ang University, Korea

The control of greenhouse gas emission is more important than ever, and accordingly, the development of a method for producing useful chemicals from CO2 feedstock with excellent technological and economic feasibility and excellent CO2 reduction ability is attracting attention. Using a continuous CO2 conversion with a heterogeneous hydrogenation catalyst, it is possible to develop a process for the efficient and selective production of Ca(HCO2)2, which has hitherto not been considered a CO2 conversion product. As a result of technical and economic analysis of the entire process, the production cost of Ca(HCO2)2 decreased by about 16% compared to the existing process, indicating a high possibility of market penetration. Through life cycle assessment, it is possible to reduce the global warming potential by about 20% compared to the existing Ca(HCO2)2 production process.

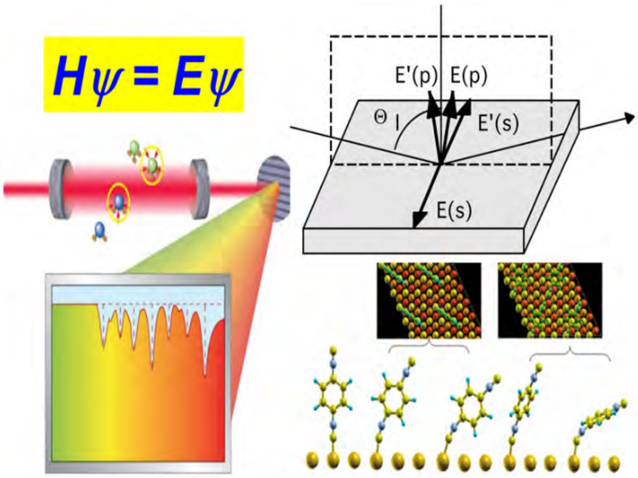
Award Lecture in Division : **PHYS1-1**
Recent Trends in Spectroscopy and Dynamics
Halla Hall THU 15:40
Chair: Tae Kyu Kim (Yonsei University)

Molecular spectroscopy at interfaces

Sang-Woo Joo

Department of Chemistry, Soongsil University, Korea

As a physical chemistry researcher, I have carried out molecular spectroscopic experiments at interfaces with my coworkers. We started to resolve quantum mechanical states of chemical intermediates in astronomy and atmosphere chemistry using high-resolution infrared laser spectroscopy. Surface chemistry at microscopic scales has been currently focused on functional materials using confocal Raman spectroscopy. We conducted experimental and theoretical studies to corroborate interfacial structures and quantify Raman scattering intensities by improving equivocal surface selection rules. Plasmonic nanostructures consisting of pure noble metals and hybrid materials can enhance Raman spectra due to their localized gap enhancements. Our Raman techniques have been utilized as an effective physicochemical tool to identify pollutants adsorbed on surfaces. Unique three-dimensional structures were prepared for selective monitoring and trace detection of hazardous species in indoor and outdoor environments. Recently, we developed a spectroscopic nanopipette probe that could estimate dynamic factors of hypoxic states in single cells. To overcome the limitations of existing phenomena caused by surface irregularities in micro and nano-sized cases, new attempts are made for controlling free electron collective oscillations in metals. We have worked toward preparing a standard substrate that can predict the Raman intensities in a more reliable way, where innovative performance is expected to replace existing methods. We humbly hope that our method can contribute to providing a small cornerstone of basic science in theragnostic biotechnology, safety monitoring and catalyst developments by applying accumulated technologies and ideas. Valuable supports and encouragements from physical chemistry community in Korean Chemical Society will be acknowledged at the meeting.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Symposium : **PHYS1-2**
Recent Trends in Spectroscopy and Dynamics
Halla Hall THU 16:10
Chair: Tae Kyu Kim (Yonsei University)

Freeze-Frame Approach for Single-Molecule Tip-Enhanced Raman Scattering (TERS) at Room Temperature.

Yung Doug Suh

Dept. of Chemistry & School of Energy and Chemical Engineering, Ulsan Nat'l Inst. of Sci. and Tech. (UNIST), Korea

Single-molecule TERS experiment in ambient conditions is of fundamental significance becausethe molecular properties can change depending on temperature and atmosphere. Specifically,understanding the conformational heterogeneity of single molecules in the non-equilibrium stateis highly desirable because it can address many fundamental questions regarding structure andfunction in many biological systems, such as protein folding and RNA dynamics. Yet,understanding the single-molecule conformational heterogeneity in ambient conditions hasremained challenging due to the rapid structural dynamics and spectral diffusions. We have performed robust hyperspectral TERS imaging of single brilliant cresyl blue (BCB)molecules in ambient conditions through the novel freeze-frame approach using a thin Al_2O_3 capping layer to suppress the spectral diffusions of single isolated molecules. Throughquantitative spectral analyses of the measured TERS spectra, we reveal the conformationalheterogeneity of single molecules. We believe this work provides an optimal protocol toinvestigate the single-molecule properties in interacting media, expanding the scope of single-molecule vibrational spectroscopy studies.

Symposium : **PHYS1-3**
Recent Trends in Spectroscopy and Dynamics
Halla Hall THU 16:30
Chair: Tae Kyu Kim (Yonsei University)

Direct probing of individual conformers by IR resonant high-resolution VUV-MATI mass spectroscopy

Sung Man Park, Yu Ran Lee[1], Chan Ho Kwon*

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea
[1]*Forensic Chemistry Division, National Forensic Service, Korea*

Conformers have similar vibrational structures both in neutral (S_0) and cationic (D_0) states. Further, the conformational equilibrium even at low temperature limits the experimental identification of individual conformers. To individually probe the conformers in equilibrium, we have developed the inventive conformer-specific vibrational spectroscopic techniques, which are based on the infrared (IR) resonant high-resolution vacuum ultraviolet mass-analyzed threshold ionization (HR VUV-MATI) mass spectroscopy. The invented IR resonant HR VUV-MATI mass spectroscopy showed their potential of becoming powerful techniques capable of measuring the identifiable vibrational spectra of individual conformers in the S_0 and the D_0 states. Moreover, we could estimate the relative populations of individual conformers using the IR dip intensity, the corresponding Franck–Condon factor, and the IR absorption cross section. Notably, our results provide indisputable experimental data regarding the conformational populations in the sense that determining the relative stability of the conformers is still immensely difficult because of the comparable force fields between the atoms in conformers. Hence, we suggest that the invented IR resonant VUV-MATI mass spectroscopy can form the basis of a very effective scheme towards conformational chemistry.

Symposium : **PHYS1-4**

Recent Trends in Spectroscopy and Dynamics

Halla Hall THU 16:50

Chair: Tae Kyu Kim (Yonsei University)

Molecular Interactions in Neurodegenerative Diseases

Sang Hak Lee

Department of Chemistry, Pusan National University, Korea

Neurodegenerative diseases, including Alzheimer’s and Parkinson’s diseases, are attributed to the accumulation of proteins, like tau and alpha-synuclein, in the brain. Many studies have shown that protein aggregates are the major cause of dementia in neurons; however, the driving force to make aggregates have not been clarified yet. Interestingly, proteins, making aggregates in cells, are either positively or negatively charged. For Alzheimer’s disease, it has been reported that the aggregated proteins are hyper-phosphorylated tau which means the proteins are highly negatively charged. Furthermore, alpha-synucleins were intrinsically negatively charged in the physiological condition. On the contrary, FUS proteins, known as the cause of Amyotrophic Lateral Sclerosis (ALS), are highly positively charged. These facts indicate that proteins cannot make aggregates because of charge imbalance. Therefore, charged proteins require counter ionic biomolecules to make aggregates. In this study, we found that small charged biomolecules, polyamine or NTP, are a critical factor in creating aggregates of charged proteins using fluorescence microscopy. Small charged molecules are bridged to interact proteins which is a molecular mechanism underlying protein aggregation.

Award Lecture in Division : **PHYS2-1**

Recent Advances in Physical Chemistry

Halla Hall FRI 09:10

Chair: Kiyoung Park (KAIST)

Computational design of the active catalyst for water splitting and energy storage materials

Do Hwan Kim

Department of Chemistry Education, Graduate School of Energy Storage / Energy Conversion Engineering, Jeonbuk National University, Korea

Rational design of an active electrocatalyst is critical for the innovative renewable energy conversion and storage technologies. By using transition metal-based catalyst, Cost-effective trifunctional catalysts have been suggested for the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR). We used density functional theory (DFT) to investigate how hierarchical design of the catalytic surface and the support layer affects the trifunctional activities. In particular, the promising catalyst significantly enhances density of states (DOS) around Fermi level, which can be estimated for the prediction of the conductivity of electrode materials. Gibbs energy of hydrogen adsorption for the HER is nearly zero, implying superior balance between adsorption and desorption of hydrogen. The oxygen evolution has lower theoretical overpotential with appropriate energy barriers in overall reaction steps. Thereby, it exhibits greater activity toward HER, OER, and ORR than conventional catalysts. This computational work is expected to create a new pathway for the research and development of cost-effective multifunctional catalysts.

Symposium : **PHYS2-2**

Recent Advances in Physical Chemistry

Halla Hall FRI 09:40

Chair: Kiyoung Park (KAIST)

Reaction Dynamics Study based on Coherent Vibrational Wavepacket Analysis

Junwoo Kim, Minhaeng Cho[1,*], Gregory Scholes[2,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Korea University, Korea*
[2]*Department of Chemistry, Princeton University, United States*

Impulsive photoexcitation of molecules generates vibrational wavepacket through the vibronic coupling with respect to the relevant electronic transition. Because the position of the wavepacket determines the average electronic transition energy of the system, the vibrational motion of a photoexcited molecule can be indirectly measured by time-resolved electronic spectroscopy. If a photoexcited molecule undergoes a photochemical reaction before photoinduced vibrational coherence disappears, the vibrational wavepackets on the reactant and the product can be observed through their transition bands, respectively. This implies that electronic and vibrational dynamics, which are associated with the photochemical reaction, can be simultaneously investigated once (1) we have sufficient time resolution for resolving high frequency vibrational motions and (2) the two transition bands indicating the reactant and product are distinguishable. Typical vibrational coherence time in the condensed phase ranges from 1 ps to 10 ps. Thus, the reaction dynamics of photoinitiated processes completing within the vibrational coherence time can be investigated by wavepacket analysis. Photosynthesis is initiated by essential ultrafast energy transfer processes after light absorption. Energy flow inside photosynthetic complexes has been widely studied by 2D electronic spectroscopy (2DES), where 2DES measures the spectral response of the complexes on a 3D space. In the presentation, 2DES-based wavepacket studies revealing nuclear motions strongly coupled to the energy transfer and relaxation processes in a bacterial light-harvesting complex are introduced.

Symposium : **PHYS2-3**

Recent Advances in Physical Chemistry

Halla Hall FRI 10:00

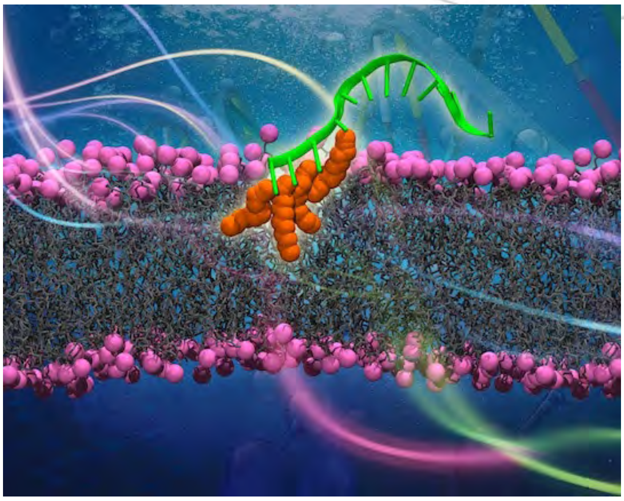
Chair: Kiyoung Park (KAIST)

Amphiphilic oligonucleotides interacting with cell membrane: experimental and computational study

Minseok Kwak*, **Sang Hak Lee**[1]

Department of Chemistry, Pukyong National University, Korea
[1]*Department of Chemistry, Pusan National University, Korea*

We studied the dynamic properties of deoxyribooligonucleotides, refer to as lipid-DNAs, which have a covalently bounded alkyl chain to uracil nucleobase. Chemically synthesized lipid-DNAs exhibit amphiphilic properties such as forming spherical micelles through microphase-separation or docking onto the cellular membrane. We employed fluorescence microscopy, be they single molecular spectroscopy as well as super-resolution imaging, to investigate the dynamics of lipid-DNAs on the lipid bilayer. In addition, we carried out computational simulations using molecular dynamics to study the dynamic details of lipid-DNAs when docking on the membrane surface. We think that the amphiphilic nature of base-modified DNAs allows materials scientists to manipulate the chemical interaction between the macromolecules and biological systems.



Symposium : **PHYS2-4**

Recent Advances in Physical Chemistry

Halla Hall FRI 10:20

Chair: Kiyoung Park (KAIST)

Direct visualization of crystallization at single-particle level using colloids

Hyerim Hwang

Chemical Engineering and Materials Science, Ewha Womans University, Korea

Crystal-liquid transitions are of the most fundamental of all processes. As they play an essential role to determine the properties of matter, there have been significant efforts to discover underlying science in these phenomena for both fundamental and technological reasons. Although an impressive body of thermodynamic data has been accumulated, the dynamics at the scale of single atoms is completely unknown.Here, we directly measure single-particle dynamics for the crystal-liquid transitions using colloids, which displays the same or similar phase behaviors as atoms or molecules do. We confine these particles and control the particle volume fraction that determines the phase behavior of colloidal suspension. We create the crystal-liquid interfaces that are at equilibrium and off-equilibrium from two different crystals. We observe the capillary fluctuations of the interfaces and extract a bulk interfacial free energy. Furthermore, we measure the attachment/detachment of particles at the interfaces which gives a unique test of crystallization kinetics.

Symposium : **PHYS2-5**
Recent Advances in Physical Chemistry
Halla Hall FRI 10:40
Chair: Kiyoung Park (KAIST)

Abnormal spatial heterogeneity in efficient perovskite solar cells and ultrasensitive near-infrared circularly polarized light perovskite detector using chiral plasmonic nanoparticles

Jong Woo Lee

Department of Applied Chemistry, University of Seoul, Korea

Two-dimensional perovskite photovoltaics have received substantial attention because of their excellent stability. In particular, it has been reported that triple-cation perovskite solar cells have higher performance and improved charge-carrier dynamics than mono-cation solar cells. Herein, we reported that abnormal heterogeneities ranging from the lateral long-range to local sub-grain scale with suppressed lattice vibrations significantly promoted charge-carrier dynamics of triple-cation perovskites [1].

As another topic, we demonstrated highly sensitive zero-biased near-infrared (NIR) circularly polarized light (CPL) detector with superior flexibility and durability [2]. In order to overcome the requirement of subsidiary optics in conventional CPL detectors, chiral molecule-incorporated low-dimensional perovskites have received attention due to the direct CPL detection capability. However, most CPL perovskite detectors confine chiroptical responses to the ultraviolet or short-wavelength visible light. Here, incorporation of chiral plasmonic gold nanoparticles (AuNPs) into the Sn-mixed perovskite enabled remarkable chirality in the NIR region with a high anisotropy factor of responsivity. Our results could provide one way to develop the ultrasensitive self-powered CPL detectors which could be used for next-generation chiral optoelectronics.

[1] Energy & Environmental Science, 14 (9), 4915-4925 (2021) “Abnormal Spatial Heterogeneity Governing Charge-Carrier Mechanism in Efficient Ruddlesden-Popper Perovskite Solar Cells”

[2] Advanced Science, 2104598 (2022) “Ultrasensitive Near-Infrared Circularly Polarized Light Detection Using 3D Perovskite Embedded with Chiral Plasmonic Nanoparticles”

Award Lecture in Division : **PHYS3-1**

Advances in AI and Theoretical/Computational Chemistry

Halla Hall FRI 14:30

Chair: Seung Kyu Min (UNIST)

Elucidating exciton-phonon cooperation in multi-chromophoric exciton migrations

Young Min Rhee

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

In a multi-chromophoric system, an exciton in one chromophore unit often migrates to another unit with a high efficiency. Of course, an exciton that is delocalized over multiple chromophore units can also migrate with a similar efficiency. Regardless of the degree of localization, the donor exciton and the acceptor exciton are not necessarily energetically degenerate. Indeed, a spontaneous exciton flow should necessarily involve an energetic bias. To satisfy the conservation law, the energy mismatch is compensated by activation or deactivation of one or more coupled phonons. How phonons and excitons combine together to achieve the high efficiency has been the target of study for a long time, and there still remains much to learn especially in naturally designed systems such as photosynthetic complexes. Here, we will discuss such cooperative aspects based on a realistically modelled photosynthetic light harvesting complex 2 (LH2). Semiclassical simulations show that vibrational coupling within chromophore units actually render any vibration quite dynamically adaptable, leading to efficient cooperation between vibrations (phonons) and excitons even in diversely varying situations.

Symposium : **PHYS3-2**

Advances in AI and Theoretical/Computational Chemistry

Halla Hall FRI 15:00

Chair: Seung Kyu Min (UNIST)

Development of new phosphorescent metal complex via deep learning

Sungmin Kim

Samsung Advanced Institute of Technology, Korea

Organic light emitting diodes (OLEDs) have become important displays over the past 2 decades due to their efficiency, flexibility, and stability. Because of their high internal quantum efficiency, phosphorescent metal complexes (PMCs) are widely used in light emitting materials and it determines efficiency, luminance, and color purity. Many PMC studies using DFT are being conducted to develop OLEDs with better characteristics. However, due to computational cost limitations, the electronic structure of PMC can be calculated only for one or two molecules, so the information that can be obtained through simulation is very limited.It is insufficient to explain complex molecular systems including electron transfer and interaction only with monomolecular calculations. Therefore, deep learning was used to overcome the limitations of DFT computation. We created a neural network-based physical property prediction model that predicts physical properties only with molecular structures based on experimental data and simulation data accumulated over the years. We also try to discover new phosphorescent metal molecules with improved performance by creating a high-efficiency generation model that can generate more than 100k molecules within a few days.

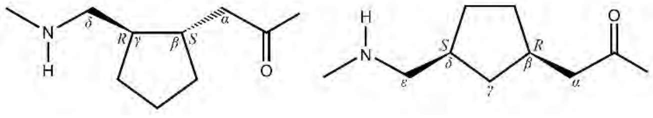
Symposium : **PHYS3-3**
Advances in AI and Theoretical/Computational Chemistry
Halla Hall FRI 15:20
Chair: Seung Kyu Min (UNIST)

Exploring Conformational Preferences of Peptide Foldamers by DFT Methods

Young Kee Kang

Department of Chemistry, Chungbuk Natioanl University, Korea

Peptide foldamers are oligomers of non-natural amino acids that adopt well-defined structural motifs, similar to those of natural peptides and proteins. It has been known that oligomers of β-, γ-, or δ-amino acid residues as well as their hybrids with α-amino acid residues can adopt various secondary structures as found in structures of peptides and proteins. For two decades, there has been a great advance in the synthesis and structural characterization of various peptide foldamers. In this talk, I will report on the conformational preferences of oligopeptides of δ-amino acid (δAc_5a) and ε-amino acid (Amc_5a) with cyclopentane substituents in the backbone investigated using DFT methods in solution. (a) The hexameric δAc_5a peptide adopted a mixed $H_{16/14}$ helical structure in chloroform, whereas the H_{14} helical structure was the most dominant conformation in water. A designed potent catalyst for organic reactions was suggested by replacing two cyclopentanes at the third and fifth residues, which are almost exactly one turn apart, of the preferred helical hexa-δ-peptide by pyrrolidines to place amine diads adjacent in sequence. (b) The Amc_5a hexamer adopted a stable left-handed (*M*)-2.3_{16} helical conformation in both chloroform and water, whereas the hexamer of Ampa (an analogue of Amc_5a with replacing cyclopentane by pyrrolidine) adopted the right-handed mixed (*P*)-$2.9_{18/16}$ helical conformation in chloroform and the (*M*)-2.4_{16} helical conformation in water. Hence, hexamers of ε-amino acid residues exhibited different preferences of helical structures depending on the substituents in peptide backbone and the solvent polarity as well as the chain length. This work was supported by the grant from the National Research Foundation of Korea. References:(1) H. S. Park and Y. K. Kang, *ChemPlusChem* **2021**, *86*, 533-539.(2) H. S. Park and Y. K. Kang, *ChemistryOpen* **2022**, *11*, e202100253.**Fig. 1** Chemical structures of δ-amino acid [2-((1*S*,2*R*)-2-(aminomethyl)cyclopentyl)acetic acid, δAc_5a] and ε-amino acid [2-((1*R*,3*S*)-3-(aminomethyl)cyclopentyl)acetic acid, Amc_5a] with cyclopentane substituents in the backbone.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Symposium : **PHYS3-4**
Advances in AI and Theoretical/Computational Chemistry
Halla Hall FRI 15:40
Chair: Seung Kyu Min (UNIST)

Chemophysical property and toxicity prediction on unknown Novichok agent candidates by using Machine Learning Model

Keunhong Jeong

Department of Chemistry, Korea Military Academy, Korea

After recent terrorist attacks by Novichok agents and following decomposition operations, one knows that how important it is to know the physicochemical properties such as vapor pressure and toxicity as well for unknown nerve agent structure. To prevent the continuous threat by new types of nerve agents, we successfully developed ML models to predict one of the most important physical property, vapor pressure to cope with the escape/removal operation when it is leaked or used. Moreover, ML classification model is successfully built on organophosphorus compounds for toxicity prediction. Importantly, tuned ML model was successfully used for predicting the toxicity of novichok materials, which is described in Chemical Weapons Convention list.

Symposium : **PHYS3-5**
Advances in AI and Theoretical/Computational Chemistry
Halla Hall FRI 16:00
Chair: Seung Kyu Min (UNIST)

The importance of a charge transfer descriptor for the screening of electrocatalysts at the example of CO_2 reduction.

Stefan Ringe

Chemistry, Korea University, Korea

It has been almost twenty years, that the linear scaling of adsorption energies of reaction intermediates in heterogeneous catalysis has started to coin the field as a blessing and a curse at the same time. It has established the possibility to construct activity volcano plots as a function of a single or two readily accessible adsorption energies as descriptors, but also limited the minimal theoretical overpotential that a catalyst can reach. In this work, we find that these established adsorption energy-based descriptor spaces are not applicable to electrochemistry, because they are lacking an important additional dimension, the Potential of Zero Charge (PZC). To reach this conclusion, we performed surface-charge dependent DFT calculations on the electrochemical CO_2 reduction to CO on various metallic surfaces, for which commonly the CO adsorption energy has been identified as descriptor. From this, we found that material trends of charge stabilization of reaction intermediates cannot be well depicted by the CO adsorption energy alone. Instead, one has to also consider the Fermi level or PZC as an additional charge-transfer descriptor, which is almost uncorrelated with the CO adsorption energy and thus effectively breaking the scaling relations. By careful comparison with published experimental data, we find the new descriptor space to rationalize experimental trends, such as the higher activity of Gold for CO production compared to Silver, but also the product selectivity for CO_2RR across various metallic and bimetallic systems. We believe that the discovery of the PZC as a critical design parameter could hold the key towards a new era of electrocatalyst design.

Award Lecture in Division : **ANAL1-5**

Recent Development of Diagnostic Virus Sensing for Post-Covid19

Room 201 THU 17:00

Chair: Sangwon Cha (Dongguk University)

In-situ Spectroelectrochemical Analysis for Interfacial Reaction Mechanism and Molecular Dynamics

Donghoon Han

Department of Chemistry, The Catholic University of Korea, Korea

Electrochemical interface is an ultrathin interfacial region between the electrode and solution where electrochemical reactions occur. The study of the electrochemical interface continues to be one of the most exciting directions in modern electrochemistry research. Much of our existing knowledge about the electrochemical interface comes from ensemble measurements and ex-situ imaging of the electrode surface. This talk describes here targets the development of a new system of in-situ spectroelectrochemical analysis that explicitly take advantage of the special characteristics of nano/micro structures, by coupling molecular transport to measurement and by exploiting the redox modulation of spectroscopic properties in organic molecules to study chemical phenomena. Now we have a comparable opportunity to create new measurement paradigms that exploit the coupling electrochemistry with time-resolved fluorescence (TRF) confocal laser scanning microscopy (CLSM) that afford a direct way to monitor such chemical reactivity as well as 3-dimensional spatial information on electrochemical reactions, in-situ and in real time.

Symposium : **ANAL1-1**
Recent Development of Diagnostic Virus Sensing for Post-Covid19
Room 201 THU 15:40
Chair: Jaebeom Lee (Chungnam National University)

Enhancement of efficiency & specificity for molecular diagnostics using nanomaterials

Tae Jung Park

Department of Chemistry, Chung-Ang University, Korea

The excellent thermal conductivity properties of nanomaterials have been used for potential applications to various fields including biotechnology during the last decades. Recently, the employment of various nanomaterials in polymerase chain reaction (PCR) produced results in significant improvement of its specificity and efficiency. In spite of their potentials and advantages to PCR technology, large surface area and their thermal and electrical conductivity of nanomaterials can provide good influences to their performance in PCR under diverse temperature conditions. This research demonstrated positive effects for the PCR efficiency and specificity of a novel nanocomposite. Some nanomaterials such as gold nanoparticles, graphene oxide, silica nanoparticles, and other forms of composites affect the improvement of thermal conductivity and heat stability. Thus, these nanomaterials led to increasing electron and thermal transfer rates and low-charge transfer resistance for the PCR reaction because thermal conductivity is an important factor in improving the PCR efficiency. When PCR was performed with these materials, the result of isothermal PCR (iPCR) and real-time quantitative PCR (qPCR) showed a great PCR specificity and efficiency to enhance the DNA amplification procedure. Therefore, it can be applied to various detection systems, and it would be suggested that a portable device for point-of-care testing will be developed to use them in situ by time and space.

Symposium : **ANAL1-2**

Recent Development of Diagnostic Virus Sensing for Post-Covid19

Room 201 THU 16:00

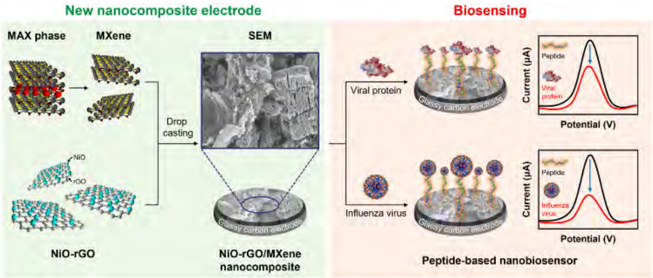
Chair: Jaebeom Lee (Chungnam National University)

Highly sensitive and selective affinity-based electrochemical biosensor for detection of influenza virus

Jong Pil Park

Department of Food Science and Technology, Chung-Ang University, Korea

Influenza is an RNA virus belonging to the family Orthomyxoviridae and it is classified into four seasonal types (A, B, C, and D) based on their antigenic differences and genetic mutation in its nucleocapsid (NP) and matrix (M) region. Among these, the A-type influenza virus can cause seasonal epidemics of the disease, resulting in severe respiratory illness worldwide. However, current diagnostic methods for influenza virus detection take a long time to achieve reliable outcomes and does not recognize the association between genetic variation and diversity. Therefore, more accurate and reliable detection methods is still challenging. In the first part of this talk, we will be showing a peptide-based electrochemical biosensor that can detect influenza viral protein and virus. The identified peptide-displaying phage clones and phage-free synthetic peptides were characterized using enzyme-linked immunosorbent assays and electrochemical analysis. To create more advanced sensor system, we fabricated nickel oxide (NiO)–reduced graphene oxide (rGO)/MXene nanocomposites and it was observed that developed nanobiosensor was capable of highly sensitive and specific detection of their corresponding influenza viruses and viral proteins with lower detection limit, better binding constant and recovery. More detailed results will be presenting in this talk.



Symposium : **ANAL1-3**

Recent Development of Diagnostic Virus Sensing for Post-Covid19

Room 201 THU 16:20

Chair: Jaebeom Lee (Chungnam National University)

Chiral Nanomaterials for Next Generation Bio-Science and Technology

Jihyeon Yeom

Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Korea

Chirality is ubiquitous in nature and is hard-wired into every living biological system. The well-known examples are L-type amino acids and D-type nucleic acids and glycans. Since the chirality of building blocks decides the handedness of assembled structures, proteins such as enzymes and receptors are also chiral. Importantly, their chiral structures are closely related to their biological properties. For example, depending on the chirality of molecules that are consumed or reach the taste buds or olfactory receptors, they taste sweet or bitter, and smell differently. These chiral-sensitive receptors are not just limited to the tongue or nose, but distributed in the stomach, intestine, and pancreas that govern overall physiology. Likewise, chirality is an important architectural consideration to build an effective artificial enzyme.

There have been enormous efforts to mimic enzymatic functionalities by developing artificial structures to utilize them under relatively harsher conditions than that in the body. However, due to the limited stability and the lack of high selectivity, it has still remained challenging. Using inorganic materials is a powerful strategy to solve these problems. Due to the thick electron clouds, inorganic materials show high catalytic activity, sensitivity, and stronger interactions with electric, electromagnetic and magnetic fields that amplify the signal. Thus, nanostructures designed with inorganic materials and biomimetic properties will offer efficient signal transition/ amplification, higher chemical and physical tolerance, and multi-functionality.

In the talk, I will convey how chiral engineering using inorganic nanostructures will provide “smart” platforms, a new level of control for drug delivery systems, tumor detection markers, biosensors, and other biomaterial based devices.

Symposium : **ANAL1-4**

Recent Development of Diagnostic Virus Sensing for Post-Covid19

Room 201 THU 16:40

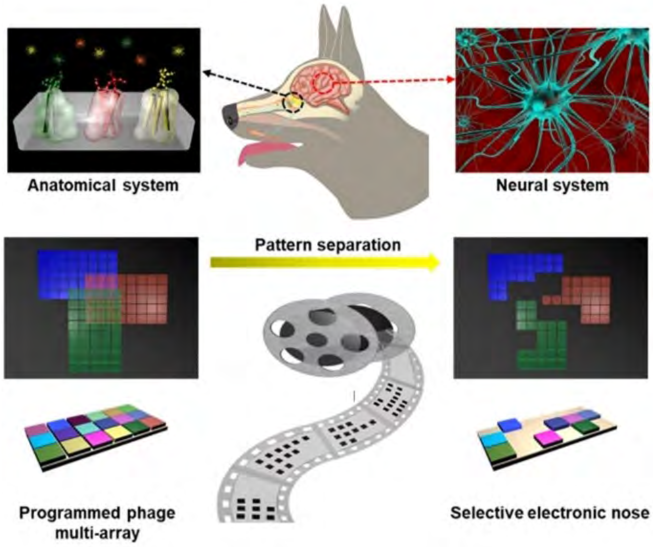
Chair: Jaebeom Lee (Chungnam National University)

Neural mechanism mimetic 2nd generation electronic nose

Jin-Woo Oh

Department of Nanoenergy Engineering, Pusan National University, Korea

From a practical point of view, the eventual dream is that the electronic nose will replace the K9-like tasks of detecting explosives, drugs, missing persons, diseases, etc. With this vision, electronic noses employing various materials and different detection methods are continuously being developed. Despite the strong potential of electronic noses, practical implementation has a hurdle to overcome. The K9 olfactory receptors incorporate up to ~ 220 million units. To realize a biomimetic electronic nose with a detection performance comparable to that of the K9, the number of the sensor units should be equal. To overcome this, understanding how K9's brain analyzes signals generated by its olfactory system is crucial. Signals generated by 220 million olfactory receptors are selectively and partially activated through the brain's learning process, called the neural pattern separation (NPS). The brain solves the pattern-learning and pattern-recognition problems of the signals it generates for complex and noisy stimuli in large and complex olfactory systems. To understand this incredible success, neuroscientists go beyond the hardware-based perspective and provide a convincing explanation based on the information processing system of the neural network. The patterns that are generated in the olfactory organs are very large and complex, and the internal method by which the brain computes patterns is not yet clear. Therefore, it is difficult to find the direct correlation between them. However, mechanism studies in olfactory organs provide clues to the selective actions that drive specific combinations of input signals. Here, by mimicking olfactory network dynamics, we developed the NPS, as shown in Figure below, and used it to develop a second-generation electronic nose. To demonstrate characteristics of the 2nd generation electronic nose with the NPS, we conducted studies that applied to a variety of applications, including polycyclic aromatic compound (PAH) detection, respiratory-based lung cancer diagnosis, and fruit freshness monitoring.


Anatomical system
Neural system
Pattern separation
Programmed phage multi-array
Selective electronic nose

Symposium : **ANAL2-1**

Recent Diagnosis and Drug Development based on Mass Spectrometry

Room 201 FRI 14:30

Chair: Jae-Min Lim (Changwon National University)

LC/MS-based analytical platform for comprehensive glycomic characterization of glycosylated biotherapeutics

Hyun Joo An

Graduate School of Analytical Science and Technology, Chungnam National University, Korea

The glycosylation of biologics is an important factor in pharmacological functions such as efficacy, safety, and biological activity and is easily affected by subtle changes in the cellular environment. Hence, comprehensive and in-depth glycomic characterization of biological products should be performed to ensure product quality and process consistency prior to regulatory approval, but it is still highly challenging due to glycan microheterogeneity produced by enzymatic machinery. High-resolution mass spectrometry (MS) has recently emerged as the premier tool for glycan analysis in biotherapeutics. Using the accurate mass measurements provided by high-resolution MS, the compositions of even large, complex glycans can easily be determined. When combined with a nano-LC separation, differentiation of structural isomers also becomes a possibility. These components, together, provide a comprehensive picture of biotherapeutic glycosylation. In this presentation, we provide an overview of MS-based analytical platform for comprehensive glycomic characterization of glycoprotein-based biotherapeutics and their biosimilars.

Symposium : **ANAL2-2**

Recent Diagnosis and Drug Development based on Mass Spectrometry

Room 201 FRI 14:50

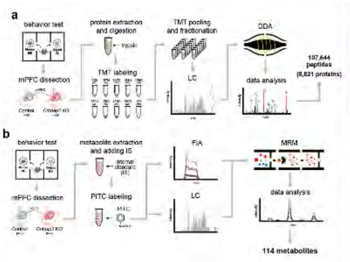
Chair: Jae-Min Lim (Changwon National University)

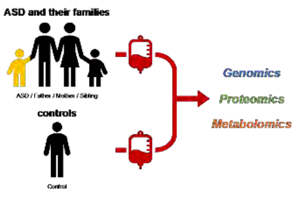
Integrative mass spectrometry analysis to discover underlying mechanisms and biomarkers for autism spectrum disorders

Min-Sik Kim

Department of New Biology, DGIST, Korea

Mass spectrometry has become a central technology in the field of biomedical research, especially for the discovery of disease biomarkers and fundamental pathophysiological mechanisms. For example, proteins and metabolites altered in tissue and blood samples from patients with diseases can be screened, identified and validated by mass spectrometry. In this lecture, I will show how mass spectrometry-based proteomics and metabolomics can be applied to discover underlying mechanisms and biomarkers for autism spectrum disorders (ASD). ASD is a major neurodevelopmental disorder in which patients present with core symptoms of social communication impairment, restricted interest and repetitive behaviors. Patients with ASD often present with medical, psychiatric, and neurological comorbidities resulting in personal, family, and social challenges. The Center for Disease Control and Prevention (CDC) in the United States has estimated that 1 in 54 children in the United States is affected by ASD. In this study, mouse models of ASD induced by a drug or a genetic mutation and blood samples from patients and their family were used to study mechansims of ASD and to discover integrative proteometabolomics-based biomarkers or ASD.





Symposium : **ANAL2-3**

Recent Diagnosis and Drug Development based on Mass Spectrometry

Room 201 FRI 15:20

Chair: Jae-Min Lim (Changwon National University)

Discovery of proteins biomarkers by high-throughput blood proteome profiling

Dohyun Han

Seoul National University Hospital, Korea

Recent improvement in high-throughput proteomic approaches have introduced new opportunities for a better understanding of these burdensome disorders and an efficient discovering of biomarkers. In this study, we discovered plasma protein biomarker candidates by a rapid and robust plasma proteome profiling strategy based on high-resolution mass spectrometry. Using optimized methods, we quantified the levels of more than 300 proteins in undepleted plasma samples of hundreds of patients. Finally, we identified a combined biomarker panel consisting of proteins using machine learning algorithm, such as a support vector machine or random forest. A high classification accuracy can be achieved by plasma proteomics in several disease models. Our approach can be helpful for accurate clinical diagnosis of various diseases. Further studies using larger, independent cohorts are needed to verify the role of these candidate biomarkers for diagnosis.

Symposium : **ANAL2-4**

Recent Diagnosis and Drug Development based on Mass Spectrometry

Room 201 FRI 15:40

Chair: Jae-Min Lim (Changwon National University)

Surface labeling with dimethylation identifies conformational changes of proteome.

Hyunsoo Kim

Convergent Bioscience and Informatics, Chungnam National University, Korea

The proper structure of protein is essential for normal functioning and performance of its role. Transformation in protein structure or conformation changes might accompany changing cleavage, binding other proteins, and interactions with the environmental molecules. Abnormal folding gives rise to defective molecular pathways and, more importantly, several diseases. A great deal of research in structural proteomics has been performed on purified proteins or protein complexes in vitro, but they were limited in their ability to examine the properties of naïve proteins in vivo and proteome-wide scale simultaneously. Here, to overcome these limitations, we suggest a strategy based on covalent protein painting (CPP). CPP is an isotopologue dimethyl labeling technique on lysine residue, which allows for the quantification of the protein folding or altered protein-protein interactions. In CPP, the accessibility value represents the proportion of protein or proteoform in which a specific lysine residue is accessible for covalent modification that is independent of the overall protein amount in the sample.

Symposium : **ANAL2-5**

Recent Diagnosis and Drug Development based on Mass Spectrometry

Room 201 FRI 16:00

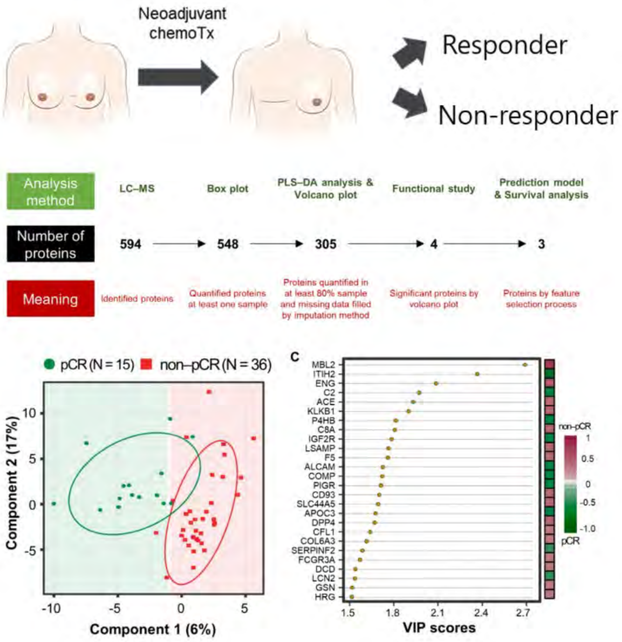
Chair: Jae-Min Lim (Changwon National University)

Clinical application of proteomics on diagnosis and therapy of breast cancer

Kyunggon Kim

Dept. of Convergence Medicine, Asan Medical Center/University of Ulsan, Korea

High resolution mass-spectrometry coupled with state-of-art protein/peptide sepatation technique have been applied on biology and translational area. And combination of other omics technology such as transctriptomics and genomics with proteomics have been extended the spectrum of its application to the precision medicine. This divergence phase of proteomics technology is playing an important and novel role as a name of proteo-genomics. At the same time, area of proteomics is reached to deep down of clincal umnet needs by not olny instrument development but also deep underatanding about the usefulness of proteomics application on translational research. Nowaday, proteomics also have been in convergence phase in clinical and translaitional area, especially in biomarker development and validation. In this presentation, I will introduce applications of clinical proteomics as a convergence aspect of proteomics and it will be presented focusing on discovery of pediction biomarkers on breast cancer. There have been clinical unmet needs to discover prognostic biomarkers to predict outcome of breast cancer prior treatment but any of the candidates showed no reliable performance. Here, proteome of plasma and FFPE tissue at the time of before treatment from breast cancer patients who showed different clinical outcomes were measured using quantitative and reproducible LC-MS platform to discover prognostic biomarker candidates to predict outcome before neoadjuvant treatment. Resulting DEPs from the FFPE tissue set and the plasma set of breast cancer patients before treatment showed the possibility of predictive biomarkers and this trial will be proceeded for verification using a large number of sample sets.



Analysis method	LC–MS	Box plot	PLS–DA analysis & Volcano plot	Functional study	Prediction model & Survival analysis
Number of proteins	594 →	548 →	305 →	4 →	3
Meaning	Identified proteins	Quantified proteins at least one sample	Proteins quantified in at least 80% sample and missing data filled by imputation method	Significant proteins by volcano plot	Proteins by feature selection process

Symposium : **LIFE1-1**

Recent Trends in Bio-Healthcare Industry

Room 203 THU 15:40

Chair: Yongwon Jung (KAIST)

Noncoding RNAs: from basic research to medical application

Younghoon Lee

Department of Chemistry, KAIST, Korea; J.R. Labs Inc., Korea

Non-coding RNAs (ncRNAs) are RNA molecules that, unlike mRNA, are not translated into proteins. They perform a variety of important biological functions in the cell. They are actively involved in regulation of gene expression at the levels of transcription, RNA processing, and translation, and even in protecting the genome from foreign nucleic acids. Most of ncRNAs act by forming base pairs with other nucleic acids. Gene silencing, a biological process in which expression of a certain gene is prevented by a base-pairing RNA molecule. We have developed several gene silencing methods and strategies to study the functions of ncRNAs. We present some examples of them in medical applications.

Symposium : **LIFE1-2**
Recent Trends in Bio-Healthcare Industry
Room 203 THU 16:05
Chair: Yongwon Jung (KAIST)

Application of deep learning models for accelerated drug discovery

Woo youn Kim

Department of Chemistry, KAIST, Korea

Computational modeling has been widely used for chemical problems in both basic science and industry. Recently, deep learning-based artificial intelligence techniques emerged as a promising data-driven approach to solve problems that cannot be tackled with conventional modeling. For example, various deep learning models have been developed for molecular design and retrosynthesis, which may lead to efficient materials and drug design. In fact, many start-ups appeared with great expectations for accelerated drug discovery. In this talk, we introduce our recent works on the development of deep learning models for drug design and virtual screening. We also demonstrate their practical applications with computational modeling in collaboration with several pharmaceutical companies.

Symposium : **LIFE1-3**
Recent Trends in Bio-Healthcare Industry
Room 203 THU 16:30
Chair: Hyun Soo Lee (Sogang University)

Molecular Modeling in Drug Discovery

Nam doo Kim

VORONOI BIO INC., Korea

In accelerating drug discovery, molecular modeling techniques have experiences considerable growth in computational powers over the last decade. Pharmaceutical industry and academic research areas are using various molecular modeling techniques for the discovery of effective drug. Nowadays, molecular modeling can be considered an integral component of the current drug discovery and development process. In structure-based rational drug design benefit significantly from understanding the essential ligand–receptor interactions for the designing a potent and effective drug that binds to the desired drug target. In this presentation, we will provide successful application towards receptor-ligand binding model predictions and hit identification study using various molecular modeling methods. In recent years, artificial intelligence tools are increasingly being applied in drug discovery. Also, we will present the application of drug development using artificial intelligence.

Symposium : **LIFE1-4**

Recent Trends in Bio-Healthcare Industry

Room 203 THU 16:55

Chair: Hyun Soo Lee (Sogang University)

Targeted Protein Degradation of p38 Mitogen-Activated Protein Kinase (p38 MAPK) as a Novel Therapeutic Approach to Alzheimer’s Disease (AD)

Nam-Jung Kim

Department of Pharmacy, Kyung Hee University, Korea

P38 MAPK (Mitogen-Activated Protein Kinase) has been considered an important target for chronic inflammatory diseases for past decades. However, targeting the kinase has not been clinically successful. Alzheimer's disease (AD) is characterized by the presence of Ab plaques and tau-aggregated neurofibrillary tangles in the brain, as well as neurodegeneration, and there is no known cure. Recent studies on the underlying biology of AD have indicated that p38 MAPK is capable of orchestrating diverse events related to AD, such as tau phosphorylation, neurotoxicity, neuroinflammation, and synaptic dysfunction. Recently, we developed a novel approach to AD by degrading p38 MAPK. In particular, p-p38 MAPK, p38 MAPK active form causing downstream activation as well as aggravating its pathology in the chronic inflammation, is selectively degraded by our approach. In addition, we confirmed that this novel approach can be effective for the treatment of AD in the in vivo transgenic mouse model.

Symposium : **LIFE1-5**
Recent Trends in Bio-Healthcare Industry
Room 203 THU 17:20
Chair: Hyun Soo Lee (Sogang University)

Novel therapeutic approaches for fibrosis: from inflammation to fibrosis and beyond

Young-Mi Lee

Senior Vice President, Head of Global R&D Innovation, Hanmi Pharm. Co., Ltd, Korea

Chronic inflammatory response induced by a variety of stimuli eventually leads into fibrosis, a progressive and ultimately fatal disease such as idiopathic pulmonary fibrosis (IPF), nonalcoholic steatohepatitis (NASH), liver cirrhosis, systemic sclerosis, and chronic kidney disease. Despite of its efforts to overcome the disease via multiple mechanism, fibrosis remains an area of high unmet clinical needs due to the lack of efficacy. Ofev (nintedanib, PDGFR/VEGF inhibitor) and Esbriet (pirfenidone, TGF-β/TNF-α inhibitor) are only two available therapies for the indication of IPF, but they can only slow the progression of the disease. Even more, there is no approved drug for NASH. To improve clinical efficacy, recent studies demonstrate advantages of targeting multiple aspects of inflammation and fibrogenesis simultaneously, by combination or multi-mode of action. Emerging data indicates that GLP-1-based therapy show anti-inflammatory effects in patients with chronic inflammatory diseases. Notably, the physiological effects mediated by activation of multiple incretin receptors could provide a robust efficacy in inflammatory and fibrotic diseases. GLP-1/Glucagon dual agonist and GLP-1/Glucagon/GIP triple agonist are currently under ongoing clinical trials for the assessment.

Symposium : **LIFE2-1**

Leading Edge Development of Genome Editing Technology and Their Applications

Room 203 FRI 09:00

Chair: Tackhoon Kim (KIST)

Single-molecule FRET studies on CRISPR-Cas12a to develop more potently engineered CRISPR genetic scissor

Sanghwa Lee

Advanced Photonics Research Institute, Gwangju Institute of Science and Technology, Korea

CRISPR-Cas12a has emerged as an attractive molecular scissor alternative to Cas9 owing to its unique features and advantages, including fewer off-target effect, an alternative PAM sequence, pre-crRNA processing, and indiscriminate single-stranded DNase activity. Notably, the indiscriminate DNase activity enables Cas12a to be used as a platform for nucleic acid detection. However, despite these advantages, Cas12a has not been well utilized as recently reported base and prime editors because it does not have complete nickase variants, unlike Cas9. Herein, we provide a thorough understanding of the mechanisms that govern the generation of complete double-stranded DNA breaks by a single catalytic site of Cas12a using single-molecule FRET assays to improve our ability to develop a rational design for more potently engineered Cas12a. This would extend the range of applications of Cas12a genetic scissor in the future.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **LIFE2-2**
Leading Edge Development of Genome Editing Technology and Their Applications
Room 203 FRI 09:20
Chair: Tackhoon Kim (KIST)

Current Status and Challenges in Genome Editing

Sangsu Bae

Department of Chemistry, Hanyang University, Korea

Genome editing tools such as ZFNs, TALENs, and CRISPR-Cas9/Cas12/Cas13 derived RNA-guided endonucleases have been broadly used for biomedical research, biotechnology, and plant transformation. CRISPR nucleases are widely exploited due to the ease of use and inexpensive cost; researchers can induce gene editing at different sites by simply altering guide RNAs. Ultimately, the Nobel Prize in Chemistry 2020 was awarded for discovering one of gene technology's sharpest tools. However, CRISPR-mediated DNA double-stranded breaks (DSBs) frequently cause unexpected large chromosomal deletions or genomic rearrangements, and also induce the p53-mediated DNA damage response. In parallel, new genome editing tools are constantly being developed. DNA base editing tools, including cytosine base editors (CBEs) and adenine base editors (ABEs), enable the direct conversion of DNA bases without producing DNA DSBs were developed. Furthermore, a prime editor (PE) that enables generating small insertion and deletion in addition to substitution of several nucleotides at target sites, was recently developed. While the gene editing mechanism is different for each tool, all tools have been developed based on the CRISPR effectors. Here I present current trends in genome editing tools along with on-going studies of my group such as development of web-based programs in CRISPR RGEN Tools (www.rgenome.net), protein engineering for enhancing specificity of base editors, and versatile application of genome editing tools for plant transformation and gene editing therapy in vivo and ex vivo.

Symposium : **LIFE2-3**

Leading Edge Development of Genome Editing Technology and Their Applications

Room 203 FRI 09:40

Chair: Tackhoon Kim (KIST)

Self-sufficient minimalism in CRISPR technology: Target with TaRGET

Yong-Sam Kim

Genome Editing Research Center, KRIBB, Korea

In spite of the developments and advancements of CRISPR technology, the present CRISPR system shows several hurdles in the clinical applications, which include patent wars between patent holders, risks in safety aspect and limitations in viral delivery. Here we introduce a new genome-editing platform, Transposase B/augment RNA-based Genome Editing Technology, termed TaRGET. We uses TnpB instead of Cas9, which is an ancestral protein for type V Cas proteins together with an engineered guide RNA, named an augment RNA. TaRGET is a self-sufficient minimalist in genome-editing technology due to its deliverability, high efficiency, persistency, high safety, and expandability. The expandability is associated with hyper-compactness of the TaRGET system, which we leveraged to create an AAV-deliverable adenine base editing system. The TaRGET-ABE system allows specific, and flexible base editing via AAV delivery in vitro as well as in vivo. We expect that these hypercompact toolsets would harness the development of in vivo gene-editing therapy and thus offer hope in life for patients with various genetic defects.

Symposium : **LIFE2-4**
Leading Edge Development of Genome Editing Technology and Their Applications
Room 203 FRI 10:20
Chair: Tackhoon Kim (KIST)

Nonviral delivery strategies of the CRISPR system for in vivo gene editing and cancer therapy

Hyun Jung Chung

Department of Biological Sciences, Korea Advanced Institute of Science and Technology, Korea

In vivo gene editing based on the clustered regularly interspaced short palindromic repeats (CRISPR) system has been challenging due to the complexity and barriers within the physiological microenvironment. We have focused on the development of efficient delivery methods of the CRISPR-associated protein 9 (Cas9) ribonucleoprotein for non-viral gene editing. We introduce a chemical tailoring approach by creating Cas9-polymer conjugates, which readily complex with single guide RNA (sgRNA) and stabilizing DNA, to form nano-assembled RNP (NanoRNP) complexes. NanoRNP shows greatly enhanced internalization and gene editing in melanoma cells in vitro, while showing low cytotoxicity. NanoRNP was designed to target PD-L1 for blockade of the immune checkpoint, which upon treatment to orthotopic melanoma model in mice resulted in major suppression of the tumor growth by modulation of the immune microenvironment. We also further developed a recombinant form of Cas9 protein by incorporation of unnatural amino acids (Cas9-UAA), which can be bioorthogonally functionalized in situ with bioactive molecules. We show that co-treatment of Cas9-UAA and antibody with chemoselective functionality allows efficient and target-specific delivery of the Cas9 ribonucleoprotein to Her2-positive breast cancer cells. We anticipate that the current strategies can be usefully applied as a therapeutic genome editing platform for treatment of various types of cancer, such as melanoma, breast cancer, and ovarian cancer.

Symposium : **LIFE2-5**

Leading Edge Development of Genome Editing Technology and Their Applications

Room 203 FRI 10:40

Chair: Tackhoon Kim (KIST)

In vivo Genome Editing for Vision

Jeong hun Kim

Ophthalmology, Seoul National University Hospital, Korea

From the FDA approval of anti-VEGF aptamer to wet-type age-related macular degeneration (AMD) of choroidal neovascularization, anti-VEGF aptamer and antibody have been widely used against all kinds of vaso-proliferative retinopathy. Actually, current therapies directed at controlling vascular abnormalities in vaso-proliferative retinopathy target VEGF and can slow the progression of these diseases. While the general role of VEGF in development has been well described, the specific function of locally synthesized VEGF in the eye is incompletely understood. Recently, RNA-guided genome surgery using CRISPR-Cas9 nucleases has shown promise for the treatment of diverse genetic diseases. Yet, the potential of such nucleases for therapeutic applications in non-genetic diseases including AMD, diabetic retinopathy (DR) as well as retinopathy of prematurity (ROP) is largely unexplored. Those vision-threatening retinopathies such as AMD, DR, and ROP are leading causes of blindness in adults and children, which is associated with retinal over-expression of, rather than mutations in, the VEGFA gene. Herein I would like to provide some my recent experimental results of therapeutic applications such as small peptide, small molecule as well as nanoparticles beyond anti-VEGF antibody. In addition, some results of in vivo genome editing in vision-threatening retinopathy would be provided.

Award Lecture in Division : **ORGN1-1**

Current Trends in Vital Molecular Imaging

Tamna Hall A THU 15:40

Chair: Min Kim (Chungbuk National University)

Multi-dimensional strategies for live cell distinction using fluorescent library

Young-Tae Chang

Department of Chemistry, Pohang University of Science and Technology, Korea

Discrimination of unique cell types in multicellular organism is the most important first step to understand the complex cell community and control their regulation. The current standard method of cell distinction is through antibodies binding to biomarkers on the cell surface. To surrogate the usage of antibodies, we have developed small organic fluorescent probes for live cell distinction. In addition to the conventional binding targets such as proteins and carbohydrates: Protein Oriented Live-cell Distinction (POLD) and Carbohydrate Oriented Live-cell Distinction (COLD), we have extended the scope of strategy to transporters, via Gating Oriented Live-cell Distinction (GOLD) and lipid composition of the cell membrane, via Lipid Oriented Live-cell Distinction (LOLD). The intrinsically complex nature of tissue requires further orthogonal strategy for higher dimension of cell discrimination. Recently, we further explored novel chemical biology approach of Metabolism Oriented Live-cell Distinction (MOLD) to enrich the toolboxes and strategy option. The design and mechanism elucidation for various immune cells will provide the new direction cell selective probe development. The multi-dimensional layer of cell distinction strategy will be the basis of characterizing extremely complex cell communities

Symposium : **ORGN1-2**

Current Trends in Vital Molecular Imaging

Tamna Hall A THU 16:10

Chair: Dokyoung Kim (Kyung Hee University)

Small-molecule two-photon probes for imaging and therapy

Hwan Myung Kim

Department of Chemistry, Ajou University, Korea

Two-photon fluorescence bio-imaging is an area of current interest, due to the many advantages this technique has over older single-photon methods. Two-photon microscopy uses photons of a near-infrared window as an excitation source of fluorophores, can result in deeper tissue images that can potentially be measured beyond a 1000 μm depth with relative stability in biological systems. With continuous development in deep-tissue optical microscopy and improvements in imaging algorithms, TPMs are gaining immense support in biomedical applications. Furthermore, it has propelled the continuous development of appropriate two-photon probes with improved sensitivities for measuring target analytes and treating abnormal specimens. In this talk, the basic TP probe design strategies and recently developed probes will be presented.

Symposium : **ORGN1-3**

Current Trends in Vital Molecular Imaging

Tamna Hall A THU 16:35

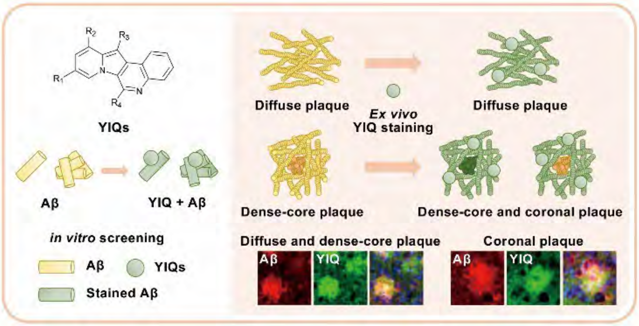
Chair: Dokyoung Kim (Kyung Hee University)

Detection of Alzheimer biomarkers by chemical sensors

YoungSoo Kim

Department of Pharmacy, Yonsei University, Korea

Detection of amyloid-β (Aβ) aggregates contributes to the diagnosis of Alzheimer disease (AD). In this presentation, novel detection methods to measure aggregated Aβ in fluid and brain by chemical sensors. The Aβ plaque levels in cortex and hippocampus are measured by either brain histology or positron emission tomography (PET). Albeit AD diagnosis dominantly relies on amyloid-PET indicating levels of insoluble Aβ plaques in the patient brain, a significant portion of subjects among the PET scan positive group are cognitively normal. Such clinical evidences, then, pointed out an urgent need to develop new biomarkers to be cooperatively used with amyloid-PET radiotracers to rule out non-demented subjects with Alzheimer's neuropathology. Recently developed Tau-PET tracers are perfect partners for amyloid-PET as tau tangles are highly associated with neurodegeneration of AD. However, a series of two PET scans is a burden for both patients and physicians for radioisotope exposures, hospitalization, and finance. Considering unrefined specificity of both amyloid- and tau-PET trances, development of innovative biomarkers can be a breakthrough technology for AD diagnosis. We found fluorescence chemicals that are available to detect monomers, dimers, oligomers, dense-core, diffuse, and coronal plaques of Aβ in the brain.



Symposium : **ORGN1-4**
Current Trends in Vital Molecular Imaging
Tamna Hall A THU 17:00
Chair: Dokyoung Kim (Kyung Hee University)

Solid-state Driven Transparent Hydrogel Fiber Formation for 3D Cell Cultures and Live Optical Imaging

Myung-Han Yoon

Division of Advanced Materials Engineering, Gwangju Institute of Science and Technology, Korea

In this research, we report solid-state crosslinking-based transparent hydrogels with controlled swelling and predefined micro/nanoscale geometry. Unlike the conventional solution-phase crosslinking utilized for highly-swollen bulk hydrogel materials, we employed i) the solid-state crosslinking between water soluble polymer and crosslinker polymer, and ii) the subsequent process for breaking physical crosslinking (e.g., hydrogen bonding) among waters-soluble polymer chains. This novel approach called hydrogelification enables both the facile definition of overall shape/dimension and the effective control over swelling ratio of the resultant hydrogel. The possible mechanisms on solid-state crosslinking and dramatic water swelling were proposed based on various characterization results. As demonstrated by micro/nanofibrillar hydrogel scaffolds prepared using electrospun nanofibers, the present method provides a novel approach to fabricate nanofiber-structured transparent hydrogel scaffolds with good biocompatibility, controlled swelling/mechanical properties, and large porosity. Finally, we demonstrate that the hydrogel nanofiber structures can be beneficial for a variety of biological applications such as 3-D cell/tissue cultures and 3-D live-cell optical microscopy imaging.

Symposium : **ORGN1-5**

Current Trends in Vital Molecular Imaging

Tamna Hall A THU 17:25

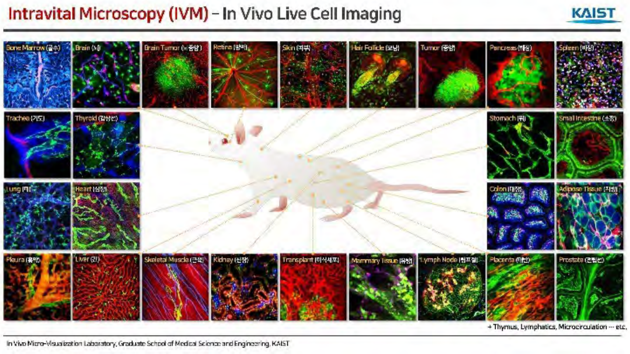
Chair: Dokyoung Kim (Kyung Hee University)

IntraVital Microscopy (IVM): In Vivo Live Animal Cellular Imaging Platform

Pilhan Kim

Graduate School of Medical Science and Engineering, Korea Advanced Institute of Science and Technology, Korea

Intravital microscopy can visualize various in vivo cellular-level dynamics such as cell trafficking, cell-to-cell or cell-to-microenvironment interactions in a live animal, providing invaluable novel insights in the dynamic pathophysiology of human diseases. During the last decade, the intravital microscopy has become a highly valuable, indispensable technique in wide areas of biomedical sciences such as immunology, neuroscience, developmental and tumor biology. Additionally, it's a unique tool for the development of new therapeutics and diagnostics by providing improved accuracy and reliability in in vivo target validation with delivery monitoring and efficacy assessment. It has been used to directly analyze the delivery and efficacy of new biopharmaceuticals such as antibodies, cell therapy, gene therapy, nucleic acids and exosome in an in vivo microenvironment. In this talk, a real-time laser-scanning intravital two-photon and confocal microscopy system will be introduced. The imaging system has been extensively optimized for in vivo cellular-level imaging of internal organs in live animal model for various human diseases, which can acquire a real-time multi-color fluorescence microscopic image in sub-micron resolution. Intravital microscopic imaging of various organs including skin, liver, spleen, pancreas, kidney, small intestine, colon, retina, lung, heart, lymph node, and bone marrow will be briefly introduced. Subsequently, recent studies utilizing the real-time intravital imaging technique to investigate dynamic cellular-level pathophysiology of various human diseases and develop new therapeutics will be introduced.



Intravital Microscopy (IVM) – In Vivo Live Cell Imaging

+ Thymus, Lymphatics, Microcirculation … etc.

In Vivo Micro-Visualization Laboratory, Graduate School of Medical Science and Engineering, KAIST

Symposium : **ORGN2-1**

Chemistry 4.0: Current Trends in Functional Organic Materials for Biomedical Applications

Tamna Hall A FRI 09:00

Chair: Woo Kyung Cho (Chungnam National University)

Coordination-Driven Approach to Grafting Organic Molecules onto Solid Surfaces for Non-Biofouling Applications

Sung Min Kang

Department of Chemistry, Chungbuk National University, Korea

Surface modification using functional organic molecules has attracted much attention owing to its potential applications in various fields including biomedical and energy conversion technologies. In these applications, efficient and robust grafting of molecules onto solid surfaces is needed because the delamination of the surface-bound molecules eventually leads to a significant decrease in its function. Herein, a coordination-driven, facile approach to graft organic molecules onto solid surfaces is reported. Briefly, solid surfaces are pre-coated by dopamine or tannic acid. Organic molecules are then grafted on the coated surfaces via Fe(III)- or Zr(IV)-mediated cross-linking reactions. This approach results in organic multilayers that suppress platelet, fibroblast, bacterial, and marine diatom adhesion on the solid surfaces. Furthermore, the molecule grafting can be selectively achieved on specific sites of solid surfaces.

Symposium : **ORGN2-2**

Chemistry 4.0: Current Trends in Functional Organic Materials for Biomedical Applications

Tamna Hall A FRI 09:25

Chair: Woo Kyung Cho (Chungnam National University)

Development of RNA therapeutics and lipid nanoparticle (LNP) formulation for in vivo delivery

Hyukjin Lee

College of Pharmacy, Ewha Womans University, Korea

In recent years, RNA therapeutics have received tremendous attention as a tool to regulate gene expression in patients. These approaches include the regulation of abnormal gene expression by short interfering RNA (siRNA) and messenger RNA (mRNA). To fully realize the potential of RNA therapeutics, an efficient in vivo delivery system is of the utmost importance. Ionizable lipid nanoparticles (LNPs) have been widely utilized for the systemic delivery of RNA therapeutics. LNPs are mainly composed of ionizable lipid or lipid like materials with helper lipid, cholesterol, and polyethylene glycol (PEG)-lipid. Although LNPs are particularly advantageous for in vivo delivery, systemic delivery of RNA therapeutics other than liver hepatocytes remains highly challenging. Ionizable lipid nanoparticles (LNPs) have been widely utilized for in vivo delivery of RNA therapeutics into the liver. However, a main challenge remains to develop LNP formulations for selective delivery of RNA into certain types of liver cells, such as hepatocytes and liver sinusoidal endothelial cells (LSECs). Here we report the engineered LNPs for the targeted delivery of RNA into hepatocytes and LSECs. The effects of particle size and polyethylene glycol (PEG)-lipid content in the LNPs were evaluated for the hepatocyte-specific delivery of mRNA by ApoE mediated cellular uptake through LDL receptors. Targeted delivery of RNA to LSECs was further investigated using active ligands. Incorporation of mannose allowed the selective delivery of RNA to LSECs, while minimizing the unwanted cellular uptake by hepatocytes. These results demonstrate that engineered LNPs have great potential for the cell type specific delivery of RNA into the liver and other tissues.

Symposium : **ORGN2-3**

Chemistry 4.0: Current Trends in Functional Organic Materials for Biomedical Applications

Tamna Hall A FRI 10:10

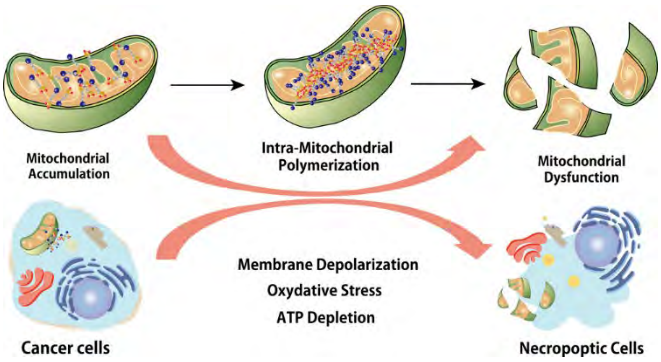
Chair: Daewha Hong (Pusan National University)

Intracellular polymerization and self-assembly to control cellular fate

Ja-Hyoung Ryu

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

The endeavor efforts to cure the cancer have been made to develop cytotoxic chemotherapy, targeted chemotherapy, to immunotherapy. However, the cytotoxic chemotherapy has severe side effects to kill healthy normal cells, and targeted chemotherapy which inhibits specific cancer proteins has a drug resistance problem, and immunotherapy is only applicable for limited patient. Therefore, it is highly demanded to develop a new paradigm of cancer therapy. Our research team has focused the efforts on the development of new cancer therapy using supramolecular approach through molecular design based on the knowledge of supramolecular chemistry. In this talk, I would like to discuss about mitochondria-targeted supramolecular therapeutics. Targeting mitochondria, the vital organelle for cell survival, has been recognized as an efficient strategy in different therapeutic techniques by disturbing the normal function. Recently, we reported that intra-mitochondrial assembly induced the dysfunction of mitochondria by disrupting the membrane, resulting in the selective apoptosis of cancer cells. In addition, we described a mitochondria-targeting biomineralization system that favorably can induce silicification and consequent apoptosis of various cancer cells. Herein, we report that the in situ disulfide polymerization inside mitochondria is based on both large accumulation of monomers (increased local concentration for polymerization) and high ROS environment (chemical fuel for disulfide reaction). During the polymerization in a mitochondrial reducing environment, the autocatalytic process enables the continuous generation of ROS and the construction of bulky structures for mitochondrial dysfunction. This in-situ polymerization shows great potential for anticancer treatment against various cancer cell lines including drug resistant cancer cell. These findings can provide a new insight into intracellular polymerization and assembly for the regulation of cellular functions and a therapeutic approach and new targeting platform for the biomedical community.


Mitochondrial Accumulation
Intra-Mitochondrial Polymerization
Mitochondrial Dysfunction
Membrane Depolarization
Oxydative Stress
ATP Depletion
Cancer cells
Necropoptic Cells

Symposium : **ORGN2-4**

Chemistry 4.0: Current Trends in Functional Organic Materials for Biomedical Applications

Tamna Hall A FRI 10:35

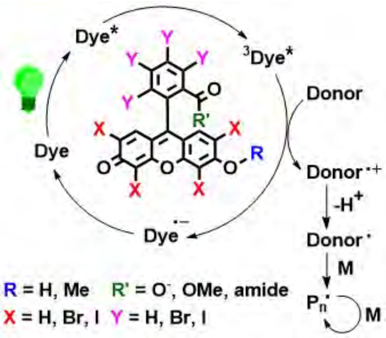
Chair: Daewha Hong (Pusan National University)

Fluoresceins dreaming beyond fluorescent probes

JungKyu Lee

Department of Chemistry, Kyungpook National University, Korea

Visible-light photoredox reactions have received much attention in various research fields, including synthetic chemistry, solar energy conversion, and cell therapy. It helps elucidate the electron transfer processes of chromophores, allows energy-efficient synthetic transformations with reduced side reactions, and contributes to developing a range of technical applications, such as dye-sensitized solar cells, CO_2 reduction, H_2 generation, and photodynamic therapy. These types of photoredox reactions provide many attractive benefits in polymer sciences because they allow the rapid photopolymerization of various vinyl compounds with low-cost equipment and radiation safety under mild reaction conditions, preventing unexpected side products. Fluorescein dyes, mainly consisting of xanthene core and phenyl ring, widely used as photoredox catalyst to initiate radical polymerization in the presence of a tertiary alkylamine (i.e., donor) under aerobic conditions. In addition, they have been explored as chromogenic and fluorogenic chemosensors for the selective detection of a target analyte as they allow rapid measurements and high sensitivity in aqueous. Herein, I present that a mechanism of photoredox catalysis using fluoresceins and its application to photoinduced radical polymerization for signal amplification.



Symposium : **ORGN3-1**

Advances in Synthetic Chemistry

Tamna Hall A FRI 14:30

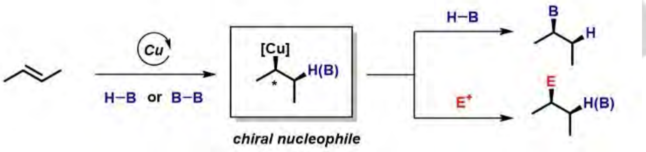
Chair: Eun Jin Cho (Chung-Ang University)

Asymmetric Reactions of Catalytic Organocopper Species for the Synthesis of Organoboron Compounds

Jaesook Yun

Department of Chemistry, Sungkyunkwan University, Korea

Development of efficient synthetic methods of organoboron compounds has attracted significant attention over the years due to their versatility in organic synthesis. In this symposium, I will present our recent progress in asymmetric tandem reactions using organocopper species, in-situ generated by addition of a chiral copper catalyst to pi-substrates.



Symposium : **ORGN3-2**

Advances in Synthetic Chemistry

Tamna Hall A FRI 14:55

Chair: Eun Jin Cho (Chung-Ang University)

Transformation of Amides using C-N Bond Activation

Sunwoo Lee

Department of Chemistry, Chonnam National University, Korea

The amide functionality is one of the key structural motifs found in biological compounds such as peptides, proteins, and alkaloids. It is also widely used to prepare agrochemicals, pharmaceuticals, polymers, and materials. Therefore, a number of synthetic routes to amides have been reported. We developed the nickel-catalyzed transamidation of unactivated secondary amides and the Claisen condensation reaction between two different amides. We also reported the amide coupling reaction with enolizable carbon nucleophiles such as ketone, ester, amides and acetonitrile to give the corresponding acylated products. In this seminar, the details about our recent findings of the C-N bond activations of amides for the synthesis of different type of acylated products will be presented.

Symposium : **ORGN3-3**

Advances in Synthetic Chemistry

Tamna Hall A FRI 15:20

Chair: Eun Jin Cho (Chung-Ang University)

Catalytic Functionalization of Normal, Undirected C-H Bonds: Recent Progress and Challenges

Soon Hyeok Hong

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The development of catalytic functionalization methods for unactivated C–H bonds has been actively pursued in our laboratory, applying both two-electron and single-electron mediated methods. A significantly improved Pd catalyst for direct C–H arylation of simple arenes was developed regarding the two-electron-based approach. Thorough mechanistic investigations, including computational studies, revealed that the Pd catalysis works via a cooperative bimetallic mechanism and the selectivity determining step is most likely a transmetallation step. For the development of novel C(sp^3)–H functionalization, metallaphotoredox catalysis via either single electron transfer (SET) or energy transfer (ET) has been applied to functionalize the challenging unactivated C(sp^3)–H bonds.

Symposium : **ORGN3-4**

Advances in Synthetic Chemistry

Tamna Hall A FRI 15:45

Chair: Eun Jin Cho (Chung-Ang University)

Recent Progress in the Total Synthesis of Indole-containing Natural Alkaloids

Cheon-Gyu Cho

Department of Chemistry, Hanyang University, Korea

We have previously demonstrated that aryl hydrazides are effective surrogates of aryl hydrazines, undergoing various reactions, including the Fischer indole synthesis to afford the corresponding indoles when treated with enolizable aldehydes and ketones in the presence of an acid. Also reported was that N-Cbz-aryl hydrazide can proceed in a Fischer indolization reaction to give N-Cbz-indole without eliminating the N-Cbz group. Recently, we have found that aryl hydrazide can be directly coupled to vinyl triflate to generate ene-hydrazide, the key intermediate in the Fischer indole synthesis. Heating in the presence of the catalytic amount of an acid effected the [3,3]-sigmatropic rearrangement reaction en route to the indole product without scrambling the regiochemistry, enabling the efficient asymmetric total syntheses of aspidospermidine and tabersonine. This new Fischer indolization base synthetic strategy has also been applied to synthesize Strychnos or uleine type alkaloids containing highly strained hexahydro-1,5-methano-1H-azocino[4,3-b]indole core, allowing the asymmetric total syntheses of uleine and tubifolidine. Presented will be our recent progress in the asymmetric syntheses of various indole alkaloids, including (-)-lundurine A, (+)-decursivine, (+)-serotobenine, and (-)-alloaritoteline.

Symposium : **MEDI1-1**
The Cutting Edge of Medicinal Chemistry
Room 302 THU 15:40
Chair: Hongchan An (KMEDIhub)

Comprehensive computational studies of membrane protein for the elucidation of mechanism of action and inhibitor discovery

Sun Choi

College of Pharmacy, Ewha Womans University, Korea

Transmembrane 4 L six family member 5 (TM4SF5) is a transmembrane protein known to interact with other TM4SFs, growth factor receptors, signaling proteins, and integrins, leading to uncontrollable cell growth and proliferation which eventually results in fibrosis and cancer. TM4SF5 contains 4 transmembrane (TM) helices, two extracellular loops (short (SEL) and long extracellular loop (LEL)), an intracellular loop, and N- and C-terminal cytosolic tails. The LEL region of TM4SF5 has previously been noted as integral to its function and interactions with molecular partners. Recently, we have identified TM4SF5 as an arginine sensor for mTORC1 activation and subsequent phosphorylation of its downstream effectors. Mutations of conserved residues in the LEL region were found to significantly affect mTORC1 function supporting the involvement of TM4SF5 in this pathway.To investigate important structural features of TM4SF5, we first generated a homology model using CD81 as template. Based on sequence conservation and mutational studies in the LEL region, we applied molecular dynamics (MD) simulations for the apo wild-type and mutant (W124A and Y126S) structures. Protein-protein docking with mTORC1 and MD simulation of ensuing complexes were also done. Trajectory and network analysis allowed us to distinguish the importance of each conserved residue to TM4SF5 structural integrity and function in the mTORC1 pathway. We also performed docking studies to predict the binding mode of L-arginine and TSAHC in the TM4SF5 LEL region. Information from the resulting protein-ligand complexes can be used for the design of potent TM4SF5 inhibitors.

Symposium : **MEDI1-2**
The Cutting Edge of Medicinal Chemistry
Room 302 THU 16:10
Chair: Hongchan An (KMEDIhub)

Targeted protein upregulation potentiates STING agonist immunotherapy

Seung Bum Park

Department of Chemistry, Seoul National University, Korea

Modulating target proteins via the ubiquitin-proteasome system has recently broadened the scope of pharmacological inventions. Stimulator of interferon genes (STING) activation is a promising strategy for immuno-oncology that promotes systemic antitumor immunity at the interface of innate and adaptive immunity. However, from the current clinical investigations of STING agonists, dysregulated STING expression or poor STING agonist pharmacokinetics pose major challenges that limit the robust antitumor response. Herein, we propose UPPRIS (upregulation of target proteins by protein-protein interaction strategy) to overcome these limitations. We discovered that the small molecule SB24011 inhibits the STING–TRIM29 E3 ligase interaction, thereby blocking the TRIM29-mediated STING degradation. SB24011 enhanced the cGAMP-mediated immunity by upregulating cellular STING levels through blocking TRIM29-induced K48 linkage-specific ubiquitination. Thus, SB24011 potentiated the immuno-oncological efficacy of cGAMP and anti-PD-1 therapy for tumor regression, confirmed in CT26 and B16F10 syngeneic mouse models. Our work successfully demonstrated that targeted protein upregulation of STING is a promising strategy for cancer immunotherapy. Furthermore, UPPRIS could be utilized to comprehend the unexplored protein-protein interaction interfaces and advance our understanding of biological processes. Overall, we anticipate that UPPRIS, an opposite approach of PROTAC, brings breakthroughs in clinical and academic research fields.

Symposium : **MEDI1-3**

The Cutting Edge of Medicinal Chemistry

Room 302 THU 16:40

Chair: Hongchan An (KMEDIhub)

Mapping the Degradable Kinome Using PROTACs

Taebo Sim

Graduate School of Medical Science, Brain Korea 21 Project, Yonsei University College of Medicine, Korea

Targeted protein degradation (TPD) such as PROTAC, AUTAC, and LYTAC is a promising and emerging therapeutic modality. Targeted protein degradation (TPD) adopting small molecule ligands utilizes ubiquitin proteasome system (UPS) or autophagy lysosomal pathway (ALP). Overactivated protein kinases caused by mutations cause various diseases such as cancer and small molecule kinase inhibitors have intensively been discovered for targeted therapy. Despite the increasing number of small molecule kinase inhibitors approved or in clinical investigations, only 7% of the human kinome has been therapeutically explored. Furthermore, despite the widespread exploration of TPD as a novel pharmacological modality, it still remains hard to predict which protein kinases are tractable and which may prove recalcitrant to this approach. In order to provide useful degrader chemical probes and clinically relevant leads across the kinome, we synthesized a variety of different kinds PROTACs of which warheads are different chemo-types of small molecule kinase inhibitors and chemoproteomic technologies were utilized to annotate the degradable kinome. Our expansive dataset provides novel PROTACs for degrading over 200 kinases. An integrated guideline for designing efficiently novel kinase PROTACs is provided by making the first map that reveals the correlation between chemical structure of the kinase PROTACs and the properties including degradability/selectivity. Moreover, novel AUTACs to degrade effectively disease-associated aggregated proteins will be briefly presented.

Symposium : **MEDI1-4**

The Cutting Edge of Medicinal Chemistry

Room 302 THU 17:10

Chair: Hongchan An (KMEDIhub)

Novel Tau-targeted Therapeutic Candidate for the Treatment of Alzheimer's Disease

Ae Nim Pae

Brain Science Institute, Korea Institute of Science and Technology, Korea

Alzheimer's disease (AD) is a late-onset, progressive, age-dependent neurodegenerative disorder. The load of neurofibrillary tangles correlates strongly with clinical progression of the disease. Although tauopathy has been extensively studied as a key hypothesis in AD, there are currently no clinical tau-targeted drugs that produce a noticeable improvement. Therefore, we studied and developed novel tau-targeted therapeutic drug candidates for the treatment of AD; in particular, tau aggregation inhibitors. We performed high-content screening based on a Tau-BiFC cell-based assay platform and identified novel tau aggregation inhibitors. Lead optimization was subsequently performed to improve potency and ADME/Tox properties, resulting in the production of DA-7503. In vivo efficacy of the candidate was validated by demonstration of memory impairment restoration in two transgenic animal models of P301L Tau-BiFC and rTg4510. The non-clinical GLP-Tox studies of DA-7503 is ongoing in order to proceed to clinical studies.

Symposium : **MEDI2-1**

Recent Trends and Advances in Small Molecule Drug Discovery (FEBPS session)

Room 302 FRI 09:00

Chair: Byeong-Seon Kim (Gyeongsang National University)

Spinal Muscular Atrophy: advancing small molecule splicing modulators from phenotypic screen to clinic

Moo Je Sung

Global Discovery Chemistry, Novartis, United States

Spinal muscular atrophy (SMA) is a debilitating genetic neurodegenerative disease and is the leading genetic cause of pediatric mortality. SMA is characterized by progressive degeneration of motor neurons, muscle wasting, paralysis, and in severe cases death. SMA is caused by the loss of the survival motor neuron 1 (SMN1) gene. A compensatory gene called SMN2 includes a single nucleotide mutation in SMN2 leading to a predominantly mis-spliced RNA transcript and an unstable truncated SMN protein which is rapidly degraded, leading to relative deficiency of SMN protein and causing disease. Several treatment modalities are currently in clinical development including gene therapy, ASO (anti-sense oligonucleotides) and small molecule SMN splicing modulators. The small molecule SMN2 splice modulator NVS-SM1/LMI070 has been found to elevate levels of full length SMN protein and extend survival in the SMN-delta-7 mouse model, and the compound is currently in Phase I/II clinical trials.

Symposium : **MEDI2-2**

Recent Trends and Advances in Small Molecule Drug Discovery (FEBPS session)

Room 302 FRI 09:30

Chair: Byeong-Seon Kim (Gyeongsang National University)

Rediscovering RON biology by its specific inhibitors

Youngshin Kwak

Discovery Research Center, LGChem Life Science Division, Korea

RON is also known as macrophage stimulating 1 receptor (MST1R) and a member of receptor tyrosine kinases, a MET proto-oncogene family. It has been reported RON is highly expressed in several epithelial tumors, promoting tumor progression and metastasis, and on macrophages surface, facilitating M2-like phenotype polarization of tumor-associated macrophages (TAM) to impair antitumor functions of CD8+ T cells.

We have identified highly RON-selective small molecule inhibitors and many efforts are underway to validate RON kinase as an attractive therapeutic target for human diseases including cancer.

Symposium : **MEDI2-3**

Recent Trends and Advances in Small Molecule Drug Discovery (FEBPS session)

Room 302 FRI 10:00

Chair: Byeong-Seon Kim (Gyeongsang National University)

Discovery and development of cevidoplenib, a highly potent and selective SYK inhibitor in Phase II clinical trials for autoimmune disorders.

Taeyoung Yoon

Oscotec, Inc., Korea

Drug discovery and development is a process through which a novel biological concept of target-disease association is interrogated and validated along the lengthy journey from benchtop to bedside. SYK (spleen tyrosine kinase) is a critical mediator of immune signals downstream of B cell receptors (BCRs), Fc receptors (FcRs), and C-type lectin receptors (CLRs). Given the biological roles partial to humoral immunity, specific inhibition of SYK is expected to address a distinct set of autoimmune disorders and/or patient subpopulations, which is juxtaposed to the currently available targeted immunotherapies such as anti-TNFa antibodies and JAK inhibitors.Cevidoplenib is a potent SYK inhibitor with an exceptional kinome selectivity currently under Phase II clinical development. In this presentation, we describe the genesis and evolution of our SYK inhibitor program along the hit-to-lead and lead optimization processes, culminating in identification of the clinical candidate. Armed with an exquisite selectivity that proved to be translated into an outstanding safety profile in Phase I clinical trial, cevidoplenib is now being tested in multiple Phase II studies for various autoimmune diseases. Some preliminary results from the proof-of-concept trials as well as our strategic rationale for further 'indication hunting' will also be presented.

Symposium : **MEDI2-4**

Recent Trends and Advances in Small Molecule Drug Discovery (FEBPS session)

Room 302 FRI 10:30

Chair: Byeong-Seon Kim (Gyeongsang National University)

Where the small molecule drug discovery should move to

Soongyu Choi

Avelos R&D Center, Avelos Therapeutics Inc., Korea

Despite its impressive response to the COVID-19 pandemic, the pharmaceutical industry is experiencing significant challenges. Drug discovery is becoming progressively more expensive – currently, it costs on average $2.6 billion to develop a single drug – and the process takes on average thirteen years. However, cancer has still absorbed the lion’s share of R&D money for years and continued to do so even as a rapidly replicating virus shook the world economy and squeezed out.Faced with questions around oncology’s dominance, industry execs often argue that the technologies and discoveries uncovered in cancer research will spread to other areas. Genomic advances and new tools are pushing more personalised, molecularly defined approaches into immunology, neuroscience and beyond. Investment into biotech and health care boomed during this pandemic as thousands of venture capital firms turned their attention to breakthrough artificial intelligence, cancer-detection technology, mental health treatments, digital doctor visits, diagnostics and more.This presentation discusses where the drug discovery industry moves to and what the VC is looking for.

Symposium : **MAT1-1**

Recent Trends in Materials Chemistry for Biomedical Applications

Tamna Hall C THU 15:40

Chair: Jin-sil Choi (Hanbat National University)

Colloidal Mesoporous Silica Nanoparticles as Bio-Adhesives for Hydrogels and Tissues

Gi-ra Yi

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

Sub-100 nm colloidal mesoporous silica (CMS) nanoparticles are evaluated as an adhesive for hydrogels or biological tissues. Because the adhesion energy is proportional to the surface area of the nanoparticles, the CMS nanoparticles could provide a stronger adhesion between two hydrogels than the nonporous silica nanoparticles. In the case of 50 nm CMS nanoparticles with a pore diameter of 6.45 nm, the maximum adhesion energy was approximately 35.0 J/m2 at 3.0 wt %, whereas the 10 wt % nonporous silica nanoparticle solution showed only 7.0 J/m2. Moreover, the CMS nanoparticle solution had an adhesion energy of 22.0 J/m2 at 0.3 wt %, which was 11 times higher than that of the nonporous nanoparticles at the same concentration. Moreover, these CMS nanoparticles are demonstrated for adhering incised skin tissues of mouse, resulting in rapid healing even at a lower nanoparticle concentration. Finally, the CMS nanoparticles had added benefit of quick degradation in biological media because of their porous structure, which may prevent unwanted accumulation in tissues.

Symposium : **MAT1-2**

Recent Trends in Materials Chemistry for Biomedical Applications

Tamna Hall C THU 16:10

Chair: Jin-sil Choi (Hanbat National University)

Supramolecular Peptide Hydrogel-Based Soft Neural Interface

Yong Ho Kim

*SKKU Advanced Institute of Nanotechnology (SAINT) & Department of Nano Engineering,
Sungkyunkwan University, Korea*

Recording neural activity from the living brain is of great interest in neuroscience for interpreting cognitive processing or neurological disorders. Despite recent advances in neural technologies, development of a soft neural interface that integrates with neural tissues, increases recording sensitivity, and prevents signal dissipation still remains a major challenge. Here, this talk introduce a biocompatible, conductive, and biostable neural interface, a supramolecular β-peptide-based hydrogel that allows signal amplification via tight neural/hydrogel contact without neuroinflammation. The non-biodegradable β-peptide forms a multihierarchical structure with conductive nanomaterial, creating a three-dimensional electrical network, which can augment brain signal efficiently. By achieving seamless integration in brain tissue with increased contact area and tight neural tissue coupling, the epidural and intracortical neural signals recorded with the hydrogel were augmented, especially in the high frequency range. Overall, our tissuelike chronic neural interface will facilitate a deeper understanding of brain oscillation in broad brain states and further lead to more efficient brain–computer interfaces

Symposium : **MAT1-3**
Recent Trends in Materials Chemistry for Biomedical Applications
Tamna Hall C THU 16:40
Chair: Jin-sil Choi (Hanbat National University)

Enzyme-free Nucleic Acid Assay via Target-mediated Formation of Quantum dot-DNA Hydrogel

Yoon Sung Nam

Department of Advanced Materials Engineering, Korea Advanced Institute of Science and Technology, Korea

For the past decades, single-stranded DNA (ssDNA)-functionalized QDs have been studied as a fluorescent probe for FRET-based DNA assays via sandwich-type hybridization as found in many publications. However, despite the superior optical properties of QDs, the limit of detection (LOD) was typically in the pM-nM range, which is not sufficient for practical applications (the aM-fM range is required). All of the works claiming the high sensitivity (~ fM LOD), in fact, employed a high-cost, time-consuming, complicated enzyme-based DNA amplification step. Unfortunately, the intrinsic sensitivity of QD-based DNA assay is still very low. Herein we present a new QD-DNA hydrogel-based FRET assay, where target DNA catalyzes the opening cycles of DNA hairpin loops tethered with a FRET acceptor into Y-shaped DNA structures, which are self-assembled with ssDNA-functionalized QDs into a hydrogel. A single target DNA mediates the self-assembly of hydrogel multiple times, and FRET pairs are placed close spatial proximity in the hydrogel network, resulting in high sensitivity for target DNA detection. As a result, the LOD of QD-DNA hydrogel is 6 fM, the lowest one ever reported without any additional DNA amplification. This LOD is about 105 times lower than the LOD of the sandwich-type assay (0.47 nM) reported in our recent work (ACS Appl. Mater. Interf. 2019, 11, 33525). The improvement in LOD is associated with the 3D hydrogel network which has benefits in placing the FRET pairs in close spatial proximity. Our assay requires 1 h to reach femtomolar sensitivity due to the synergetic effect of efficient 3D FRET and target DNA-catalyzed amplification. This new DNA assay also has excellent specificity with single-base mismatch discrimination in ~ 10 min.

Symposium : **MAT1-4**

Recent Trends in Materials Chemistry for Biomedical Applications

Tamna Hall C THU 17:10

Chair: Jin-sil Choi (Hanbat National University)

Nanotechnology-Enabled Neural Stimulation

Jae-Hyun Lee

NanoBiomedical Engineering, Yonsei University, Korea

Nanotechnology has been served as a platform technology in various field of researches, especially enabling interfacial sciences between nanoscale materials and biological systems. This talk covers two important nanomaterials, i.e., silicon nanowire and magnetic nanoparticle, and their utilization as a probe for addressing and stimulating neuronal cells. Firstly, use of the semiconducting nanowires enables nanoscale field effect transistor devices which were demonstrated to probe electrophysiological behaviors with sub-cellular resolution of precision in cultured neurons. Secondly, use of the magnetic nanoparticles enables generation of mechanical force in a remote setting which works as physical stimuli to activate mechanotransduction systems in biology non-invasively. These approaches are comparable to optogenetics in terms of using physical stimuli to control neuronal behaviors. I would like to deliver that the nanotechnology is beneficial for controlling biosystems in single cell level, which would potentially advance current biology to decipher veiled cell networks and to treat diseases.

Symposium : **MAT2-1**

Synchrotron Radiation Based Development and Analysis of Advanced Materials

Tamna Hall C FRI 09:30

Chair: Dae-Hwan Park (Chungbuk National University)

Ni, Co, Mn L_3-edge x-ray absorption spectro-nanoscopy study on $Li_xNi_{0.88}Co_{0.08}Mn_{0.04}O_2$ primary particles

Hyun-Joon Shin

Physics Department, Chungbuk National University, Korea

$Li_xNi_{0.88}Co_{0.08}Mn_{0.04}O_2$ primary particles for lithium-ion battery (LIB) cathode materials were investigated by using an x-ray absorption spectro-nanoscope, scanning transmission x-ray microscope (STXM), at Pohang Light Source. Space resolution of the STXM was 30nm. Space-resolved L_3-edges of the Ni, Co, and Mn ions and O K-edge spectra were obtained to investigate the oxidation number and chemical states of ions of each element inside the primary particles. Spectro-nanoscopic data were obtained from the particles with differently charged states and at differently annealed temperatures upto 800 °C.In the experiment on pristine and charged (4.35 V at 1st cycle charge) states particles, averaged oxidation number of the Co and Mn ions were +3, and +4, respectively, throughout the particles for both charge states; while that of the Ni ions was about +2.5 for pristine and +3.2 for charged states; and the values were lower for smaller size particles and outer area of the particles. In the experiment of high-temperature annealing, primary particles with average oxidation number of +3, +4, +3, respectively for Co, Mn, Ni ions, at room temperature were investigated. At 200 °C, the average oxidation numbers of the Co and Mn ions were basically the same as those at RT, and those of the Ni ions were between +2 and +3. At 400 °C, the average oxidation numbers of the Ni and Co ions decreased to +2, whereas that of the Mn ions was +4. At 600 °C, the Ni, Co, and Mn ions were all strongly reduced; the Ni ions were mostly in the metallic state, the Co ions comprised a mixture of the metallic and +2 oxidation states, and the Mn ions were reduced to +2 oxidation number. The spectral images indicated that the Mn ions, compared to those of the Ni and Co ions, developed strong phase changes within the particles. At 800 °C, strong morphological changes occurred, with the Ni and Co ions mostly in the metallic state, and with the Mn ions predominantly +2 oxidation number.

Symposium : **MAT2-2**

Synchrotron Radiation Based Development and Analysis of Advanced Materials

Tamna Hall C FRI 09:50

Chair: Dae-Hwan Park (Chungbuk National University)

Structural studies of energy materials using synchrotron X-ray techniques

Tae Joo Shin

Graduate School of Semiconductor Materials and Devices Engineering, Ulsan National Institute of Science and Technology, Korea

In order to solve issues such as sustainable energy sources, there is an urgent need for the development of eco-friendly and efficient energy conversion and energy storage materials. Structure-property relationship make structural analysis more important and a new paradigm is urgently needed to accelerate the real-time measurements, on-line structural analysis, and new material design and synthesis processes. In the presentation, the research results in the field of solar cells and batteries using synchrotron X-ray techniques will be discussed.

Symposium : **MAT2-3**

Synchrotron Radiation Based Development and Analysis of Advanced Materials

Tamna Hall C FRI 10:10

Chair: Dae-Hwan Park (Chungbuk National University)

Manipulating phase transformation during electrochemical reactions: lithium-ion batteries and battery-inspired electrocatalysis

Jongwoo Lim

Division of Chemistry, Seoul National University, Korea

Electrochemically dynamic environment in lithium-ion batteries and water electrolysis often makes phase transition of electrode unpredictable. Lithium-ion insertion kinetics fundamentally hinges upon phase transformation behavior during (dis)charging at high cycling rates. Ni-rich NCM, one of the most widely investigated cathodes, shows strong phase-separating behavior as cycling rate increases. However, the origin of phase separation remains unclear and inconsistent, complicating quantitative analysis. On the other hands, surface reconstruction of electrocatalysts during water electrolysis determines the active species and the catalytic performance. However, rationally modulating the dynamic surface restructuring and generating active surface species remain tremendous challenges. In the first part of my talk, I will present how we can redirect the detrimental two-phase behavior to single-phase at a fast cycling rate during lithium-ion battery operation. Electrochemically manipulating the lithium-ion distribution within the NCM particles could effectively induce facile lithium diffusion and solid-solution phase behavior. The second half of my talk will present a novel cationic redox-tuning method to redirect the in-situ surface reconstruction of a transition-metal-oxide electrocatalyst for the oxygen evolution reaction (OER). Cl-doping lowered the potential to trigger in situ cobalt oxidation and lithium leaching, which induced the surface of LiCoO1.8Cl0.2 to transform into a self-terminated amorphous (oxy)hydroxide phase during the OER. We further demonstrated that surface-restructured LiCoO1.8Cl0.2 outperformed many state-of-the-art OER catalysts and demonstrated remarkable stability

Symposium : **MAT2-4**

Synchrotron Radiation Based Development and Analysis of Advanced Materials

Tamna Hall C FRI 10:30

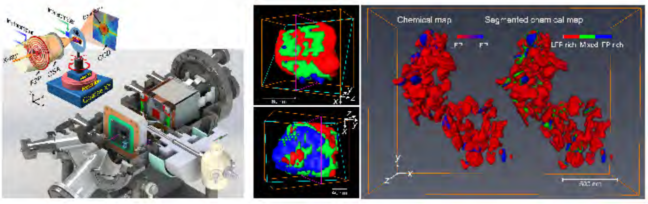
Chair: Dae-Hwan Park (Chungbuk National University)

A new era of quantitative analysis for chemically heterogeneous nanomaterials: STXM & Ptychography

Young-Sang Yu

Department of Physics, Chungbuk National University, Korea

Visualization capable of nonequilibrium chemical states and their morphologies at proper spatial/spectral resolution is central to elucidating the complex phenomena in nanomaterials that underpin materials' properties. These observations need to provide quantitative information at multiple scales, including the single-particle level, where incomplete reactions and failure at the required length and time scales are prone to occur. Scanning transmission X-ray microscopy (STXM) combined with high-brightness X-ray synchrotrons is an ideal tool to probe a wide variety of contrast mechanisms for studying material properties. However, it has been limited in spatial resolution to many times the X-ray wavelength by the nature of X-ray focusing optics. X-ray ptychography, on the other hand, has been developing as a kind of coherent X-ray scattering-based imaging scheme. The scattering from the sample as a function of X-ray source brightness and wavelength only limits achievable spatial resolution under an ideal instrumentation condition. This talk will present recent accomplishments to adapt STXM & ptychographic imaging at the Advanced Light source (ALS). The main objectives are to explore and develop a multimodal, multidimensional, and multi-length scale methodology to follow the chemical and microstructural evolution at the nanoscale. Our efforts for demonstration of multidimensional, multilength scale, and multimodal visualizations will allow spectro-microscopy with faster data acquisition rates in OASIS (Ochang Advanced Synchrotron for Industry and Science) to perform dynamic 3D measurements over larger field-of-view, with higher spatial resolution, under specific sample environments, such as varying temperature, applied voltage, or other-directed influences.


X-ray
FZP
OSA
CCD
Chemical map
Segmented chemical map
LFP rich
Mixed
FP rich
X
Y
Z

Symposium : **MAT3-1**

Metallization Process for Semiconductor and Electronic Devices

Tamna Hall C FRI 14:30

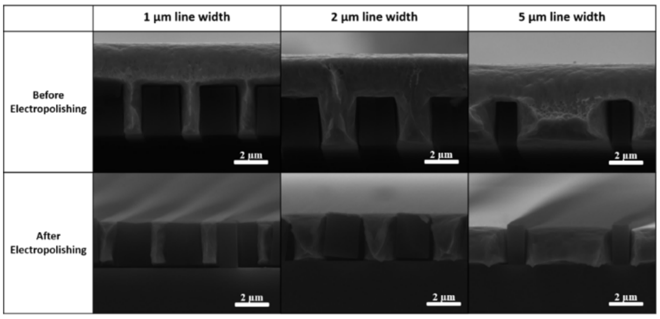
Chair: Myung Jun Kim (Kyung Hee University)

Electrochemical Polishing of Cu for the Redistribution Layer on Fan-Out Wafer Level Packaging

Bongyoung Yoo

Department of Material Science and Chemical Engineering, Hanyang University, Korea

The Fan Out Wafer Level Packaging (FOWLP) has become increasingly important for the compact and high performance electronic devices due to the advantages that low packaging cost, enhanced packaging capabilities, and a large number of Input/Output (I/O) counts. In the FOWLP process, the fabrication of the Cu Redistribution Layer (RDL) was one of main process for the FOWLP. This process was conducted by following steps; trench Cu filling and Chemical Mechanical Polishing (CMP) of overburden Cu layers during the Cu filling. However, this CMP process caused an increase in process cost therefore alternative methods are required.Electrochemical Polishing was a process that makes surface of the conductive substrate smooth when it was anodically polarized in the electrochemical polishing solutions. Generally, electrochemical polishing of copper was conducted in phosphoric acid and it has been investigated from many researchers. Polishing effect can be observed within the potential range where the limiting current density plateau in the polarization curve. This method has advantages that simple and cost-effective method therefore it can be used for Cu removal replacing CMP method.In this research, ECP was used for removing overburden Cu layers deposited on patterned substrate. Electrochemical behavior of ECP was studied by cyclic voltammetry and the ECP behavior at various polishing conditions such as applied potential, charge density and electrolyte concentration, was investigated.


1 µm line width
2 µm line width
5 µm line width
Before Electropolishing
After Electropolishing
2 µm
2 µm
2 µm
2 µm
2 µm
2 µm

Symposium : **MAT3-2**

Metallization Process for Semiconductor and Electronic Devices

Tamna Hall C FRI 15:00

Chair: Myung Jun Kim (Kyung Hee University)

Development of superb copper electroplating solution for micro-bump : SmartPlate^{TM} series

Min Hyung Lee

Heat & Surface Technology R&D Department, Korea Institute of Industrial Technology (KITECH), Korea

A superb copper electroplating solution, SmartPlate^{TM} series, was developed in order to improve the process performances of Cu electroplating for sub-50 um micro-bump. SmartPlate^{TM} series shows the world’s best performances in terms of plating speed, bump shape and Kirkendall voids, which are the key performances of copper plating in micro-bump. The electroplated Cu bump using SmartPlate^{TM} series shows thickness non-uniformity less than 3 % even at the high electroplating speed of 3um/min, which was achieved by using a unique combination of organic additives including shape-inducing agents in SmartPlate^{TM} series. The Kirkendall voids at the Cu/solder interface could be reduced over 90 % by the implementing the optimized shape-inducing agents in SmartPlate^{TM}.

Symposium : **MAT3-3**

Metallization Process for Semiconductor and Electronic Devices

Tamna Hall C FRI 15:30

Chair: Myung Jun Kim (Kyung Hee University)

Electrochemical metallization process for interconnection

Jae-Hong Lim

Department of Materials Science & Engineering, Gachon University Global Campus, Korea

Electrochemical process has been attracting attentions because of its many advantages including low-cost, rapid deposition rate, and ease of control their microstructure and crystallinity by adjusting electrochemical parameters. Among many applications, electrochemical deposition techniques can be used for interconnection in semiconductors. The durability or efficiency of the device is degraded due to heat generation. It is necessary to effectively release the generated heat. Based on demands for modern heat sink printed circuit board (PCB) manufacturing, the robust and reliable plating technique of PCB is necessary. In addition, many electronic devices need low resistive and reliable contact for high performance. Electrochemical process for these applications will be presented.

Symposium : **MAT3-4**

Metallization Process for Semiconductor and Electronic Devices

Tamna Hall C FRI 16:00

Chair: Myung Jun Kim (Kyung Hee University)

Monitoring and control of highly reactive species in Cu electroplating bath

Seunghoe Choe

Electrochemistry department, Korea Institute of Materials Science, Korea

Copper electrodeposition is one of the core processes for manufacturing semiconductor devices, printed circuit boards, and copper foils. Cu plating bath typically contains a small amount of organic additives for controlling the properties and morphology of the electrodeposited film, which have been referred as accelerator, suppressor, and leveler according to their roles. However, these additives could be decomposed via chemical and electrochemical reactions during electroplating process, which leads to irreversible degradation of bath. Therefore, it is needed to exam the mechanism of additive decomposition, monitoring methods for prediction of bath condition, and advanced tool to suppress the additive decomposition. In this presentation, we will briefly introduce the mechanism of additive decomposition, and its effect on the performance of bath. Also, we will present the detection of reactive species (Cu+, free-chlorine) that cause decomposition of additives, and present how to suppress the formation of them, which includes the use of radical scavenger or sacrificial polymer coating.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **ELEC1-1**

New Horizons in Molecular Electrochemistry for Energy Storage Systems

Room 402 THU 15:30

Chair: Hye Ryung Byon (KAIST)

Coupling spontaneous chemical reactions with advanced energy storage systems

Minah Lee

Korea Institute of Science and Technology, Korea

The organic compounds hold the boundless potential for enriching the chemistry of energy storage technologies. In this talk, I will first present utilizing chemical charge transfer reactions of redox molecules for a battery manufacturing process, called chemical prelithiation, to compensate for the loss of active Li during the initial cycling of batteries. Our recent work using tailored Li–arene complexes will be covered, which provides unparalleled reaction homogeneity and simplicity compared to other methods. [1, 2] I will also discuss chemical activation strategies to facilitate electrochemical multivalent metal cycling.[References]1. M. Lee et al., Angewandte Chemie Int. Ed. 59, 14473 (2020) 2. M. Lee et al., Journal of the American Chemical Society. 143, 9169 (2021)

Symposium : **ELEC1-2**
New Horizons in Molecular Electrochemistry for Energy Storage Systems
Room 402 THU 15:55
Chair: Hye Ryung Byon (KAIST)

Permselective nanoporous membranes by polymerization-induced microphase separation

Myungeun Seo

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

A membrane should be able to regulate transport across the membrane and achieve selective permeation of target substances while rejecting undesirables. For instance, facilitating proton conduction while suppressing vanadium crossover is critical in the vanadium redox flow battery membrane. A nanoporous polymer membrane derived from a block copolymer precursor can be used as an ideal model system, as well-defined and surface-tailorable pores can be produced with control over pore size. In this talk, I will highlight our recent progress in fabrication of such nanoporous membranes via the polymerization-induced microphase separation (PIMS) process. I will discuss how to control the domain size and surface functionality in the PIMS process towards fabrication of permselective membranes.

Symposium : **ELEC1-3**

New Horizons in Molecular Electrochemistry for Energy Storage Systems

Room 402 THU 16:20

Chair: Hye Ryung Byon (KAIST)

Polymer Design for Energy Storage Devices

Soojin Park

Department of Chemistry, Pohang University of Science and Technology, Korea

Although lithium-ion batteries (LIBs) are used in various fields, such as small devices and electric vehicles, the low cycling stability due to the acceleration of salt degradation at high temperatures remains a significant challenge. The batteries are typically assembled in a dry room that controls moisture because lithium salts in the electrolytes are highly reactive with moisture, which has a significant effect on the battery performance. In this talk, impurity scavenging separator membrane (ISM) was fabricated using a powerful H2O and HF scavenging material. This material was synthesized by an urethane reaction between porous silica (p-SiO2) and (3-isocynatopropyl)triethoxysilane (ICPTES). The p-SiO2 reaction with ICPTES suppressed the acidification of the electrolyte with water and resulted in maintaining the shape of the SiO2 particles. The multifunctional separator exhibited high capacity retention of 87%, 79%, and 74% at various electrodes including LiMn2O4 (LMO)//Li4Ti5O12 (LTO), Li[Ni0.8Co0.1Mn0.1]O2 (NCM)//Graphite, and LMO//Graphite, respectively, at high temperature (55℃). In addition, I present a a facile but efficient way of incorporating the natural polymers with an ionically conductive crosslinker, which can construct a robust network for silicon anodes. The boronic acid in the crosslinker spontaneously reacts with natural polymers to generate boronic ester at room-temperature without any kind of triggers, which gives a strong and dynamic covalent bonding to the supramolecular network. The other component in the crosslinker, polyethylene oxide, contributes to the enhanced ionic conductivity of polymers, leading to the outstanding rate performances even at a high mass loading of silicon nanoparticles (>2 mg cm-2).

Symposium : **ELEC1-4**

New Horizons in Molecular Electrochemistry for Energy Storage Systems

Room 402 THU 16:45

Chair: Hye Ryung Byon (KAIST)

Molecular chemistry for advanced battery separators

Sang-Young Lee

Department of Chemical and Biomolecular Engineering, Yonsei University, Korea

Rechargeable Li-batteries have ceaselessly garnered a great deal of attention, with rapid growth of emerging application fields such as smart portable electronics, electric vehicles, and grid-scale electricity storage systems. Taking into an account that a key factor governing battery performance is how to facilitate ion and electron transport, roles of battery separator (membranes) should not be underestimated. Currently, most widely used battery separators are based on polyolefin materials. These porous polyolefin separators have several advantageous attributes suitable for practical use in Li-ion batteries. However, their intrinsic limitations stemming from the chemical/electrochemical inertness often raise significant concerns related to ion transport (cell performance) between the electrodes, which becomes more serious at emerging battery systems such as high-energy-density Li-ion batteries based on high-Ni cathodes and Si anodes, Li-sulfur, and Li-metal batteries. In this talk, we present a class of advanced battery separator strategies based on molecular chemistry control as well as customized porous structure, including functional group-modified cellulose nanofibrils which can chelate heavy metal ions dissolved from cathodes and polysulfides generated from sulfur cathodes, surface-modified nanoparticles for use in ceramic separators, and covalent organic framework-based porous ion conductors with directional ion channels. Notably, these new separators with the well-tailored molecular chemistry exhibit improvements in electrochemical performances (in particular, cyclability) of cells while ensuring facile and uniform Li-ion flux toward electrodes, which lie far beyond those achievable with commercial polyolefin separators.

Symposium : **ELEC1-5**

New Horizons in Molecular Electrochemistry for Energy Storage Systems

Room 402 THU 17:10

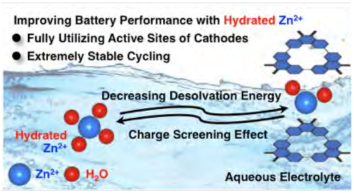
Chair: Hye Ryung Byon (KAIST)

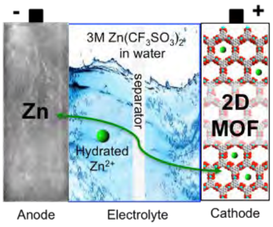
Hydration Effects and Emerging Materials for Divalent Batteries

Kwan Woo Nam

Division of Chemical Engineering and Materials Science, Ewha Womans University, Korea

The battery community is paying increasing attention to post Li-ion batteries, which can transcend current Li-ion batteries with respect to key electrochemical properties, cost, and safety. As promising alternatives, divalent batteries such as Mg and Zn are gaining considerable attention since they can take advantage of increased capacity resulting from the divalent charge of their carrier ions. In addition, they are cost-effective, environmentally benign, and subject to reduced fire hazards. Mg and Zn batteries, however, still linger at the research stage, requiring cathode materials with enhanced performance. The main challenge in developing the cathode materials of divalent batteries is associated with the dual positive charge that induces stronger electrostatic interactions with the host framework, impeding the diffusion of divalent ions. The presence of these positively charged metal ions also imposes a higher dehydration energy penalty when divalent ions pass through the electrode-electrolyte interface, constituting an additional barrier in the overall cell operation. In this presentation, I would like to briefly the hydration effects in the host cathode and interface between the cathode and electrolytes: (1) the charge-screening effect by crystal water in the host cathode and (2) the lowering of desolvation energy by intercalation of hydrated divalent ions at the electrode-electrolyte interface. Furthermore, the main part of this talk will cover the development background and reaction mechanism of two emerging materials—redox-active organic macrocycle (PQ-Δ) and conductive 2D MOF—which have recently been introduced as aqueous Zn-battery cathode materials. In addition, the role of hydration effects in the PQ-Δ and MOF cathodes will be explained in detail.





129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Symposium : **ELEC2-1**

Recent Developments and Future Issues in Physical and Analytical Electrochemistry

Room 402 FRI 09:00

Chair: Byung-Kwon Kim (Ewha Womans University)

Plasmonic monitoring with electrochemistry in photocatalytic reaction and electrochromism

Jeong-Wook Oh

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Plasmonic nanoparticles have been of particular interest due to their characteristic and controllable optical properties that can be useful for various optical signal enhancements and photocatalytic reactions. Plasmonic behavior originates from the collective oscillation of free electrons in plasmonic materials. We monitored and analyzed the plasmonic behavior in photocatalytic reaction and electrochromic behavior using electrochemical measurements. We demonstrated a plasmon-enhanced catalytic reaction with Pd/Au bimetallic structure and observed electrochromic behaviors of Au nanocubes with varying electrical potential, which was monitored by in-situ dark-field microscopy.

Symposium : **ELEC2-2**

Recent Developments and Future Issues in Physical and Analytical Electrochemistry

Room 402 FRI 09:25

Chair: Byung-Kwon Kim (Ewha Womans University)

In Situ Monitoring of Single Droplet Collision

Jun Hui Park

Department of Chemistry, Chungbuk Natioanl University, Korea

We describe a simple method for real-time observation of collision and recollision behavior of a single aqueous attoliter droplet in an organic solvent through single-entity electrochemistry. The dynamics and morphology of the droplet after the collision event at the Au ultramicroelectrode (Au-UME) were monitored by consecutive cyclic voltammetry and amperometric current−time measurements. By sequentially applying oxidative potential and reductive potential at the Au-UME in the presence of attoliter droplets containing reversible redox species (e.g., ferrocyanide), we successfully detected the oxidative collision spike and its reductive recollision spike successively owing to the reversible redox reactions inside the droplet. Because the redox species was dissolved in a reduced form, the reductive collision spikes observed are the direct evidence that the water droplets colliding at the electrode surface are detached after the oxidation reaction. The collided droplet properties, such as size change and contact area, are also investigated and discussed. These instructions are an example of what a properly prepared.

Symposium : **ELEC2-3**

Recent Developments and Future Issues in Physical and Analytical Electrochemistry

Room 402 FRI 09:50

Chair: Byung-Kwon Kim (Ewha Womans University)

Application of SECM(Scanning Electrochemical Microscopy) in the Development of Electrochemical Hydrogen Production and Storage Technology

Hyun S. Park

Hydrogen Fuel Cell Research Center, Korea Institute of Science and Technology, Korea

Scanning Electrochemical Microscopy (SECM) is the analytical technology to investigate the surface of conductors or insulators using ultramicroelectrode probe. In this presentation, the application of SECM is discussed in the development of electrochemical hydrogen production and storage technology. The use of hydrogen as an energy vector of renewable power sources is accepted as the essential way to construct new industrial structure without significant green-house gas emissions. Hydrogen can be produced by many methods including fossil fuel reforming, thermo- or photochemical, and electrochemical water splitting. Among them, water electrolysis using renewable electricity from solar or wind power is considered as the cleanest production process to make ‘green hydrogen’. Along with the green hydrogen production, economically efficient storage of the hydrogen in the foam of liquid organic hydrogen or ammonia is pursued to reduce the cost of longer and larger storage and transportation of the energy carrier. The production of ammonia can also be performed in electrochemical processes, so to avoid the carbon emission from thermochemical nitrogen hydrogenation reactions. In this presentation, a practical use of SECM is discussed in the development of water oxidation electrodes and electrochemical nitrogen reduction catalysts. It includes the required research topics to further enhance the technical and economic efficiency of green hydrogen production and storage devices.

Symposium : **ELEC2-4**

Recent Developments and Future Issues in Physical and Analytical Electrochemistry

Room 402 FRI 10:15

Chair: Byung-Kwon Kim (Ewha Womans University)

Mixed potentials under isochoric processes in composite electrodes.

Heung Chan Lee

Battery Material Lab, Samsung Advanced Institute of Technology, United States

Electrochemical processes of recent battery electrodes are becoming more complicated as more species are added for higher battery performances. Various active materials with different redox states varying their volume and pressure involve complex mixed potential situation. For example, silicon-graphite composite anode, which has been known as a quite successful route to circumvent the downside, large volume change, while maintaining the advantage, high energy density, of silicon. Also, in an all-solid state battery, volume change of active materials and their consequent pressure change will affect overall electrochemical responses of the system. The fundamental electrochemical interactions between active materials with their dynamic mechanical response with consequent pressure/volume changes have not been well understood. Here, some of recent efforts to elucidate the electro-chemo-mechanical processes of composite electrodes will be presented. It includes operando x-ray diffraction analysis, volume and pressure measurement under chrono-amperometric and chrono-potentiometric processes, and other spectroscopic and microscopic analysis that conclude strong dependencies of form factors and ratios of the active materials on the complex processes of composite electrodes.

Symposium : **ELEC2-5**

Recent Developments and Future Issues in Physical and Analytical Electrochemistry

Room 402 FRI 10:40

Chair: Byung-Kwon Kim (Ewha Womans University)

Flash-photolysis time-resolved microwave conductivity measurement (a microwave-based pump-probe spectroscopy) and photoinduced free-carrier dynamics

Jaehong Park

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

For molecular optoelectronics, photoinduced generation and recombination dynamics of free-carriers (mobile electrons and holes) are the key process of the device operation, for example organic photovoltaics. To probe this dynamics, various spectroscopic and electrical techniques have been utilized. In this presentation, I will discuss flash-photolysis time-resolved microwave conductivity (FP-TRMC) measurement, an X-band microwave-based pump-probe experimental technique. First, my presentation will introduce several demonstrative studies utilizing FP-TRMC techniques, highlighting its unique features such as electrode-less and non-invasive measurements as well as extremely high sensitivity that enables to detect photoinduced carrier dynamics under 1-sun condition. Second, my presentation will discuss the new opportunities that the complementary conventional pump-probe transient absorption spectroscopy and FP-TRMC can provide to elucidate photophysical phenomena relevant carrier-generation and recombination processes.

Symposium : **EDU-1**
Current Trends in Chemistry Education
Room 301 THU 15:40
Chair: Hyun-Ju Park (Chosun University)

2022 revised science curriculum focused on chemistry

Wonho Choi

Department of Chemical Education, Sunchon National University, Korea

The 2022 revised curriculum is being created under the goal of cultivating sustainable society and digital literacy. The achievement standards of the curriculum were organized to be operated for 16 weeks for the autonomous operation of the school curriculum, and the number of units was adjusted so that elementary and middle schools could operate career-linked semesters in the last semester. The material area of elementary school science consists of 7 units: properties of material, state change of water, properties of gas, dissolution and solution, separation of mixtures, acid and base, and change of material. The material area of middle school science consists of 5 units: state change of matter, properties of gases, characteristics of material, composition of material, and regularity of chemical reactions. High school science subjects include ‘integrated science’, ‘science inquiry experiments’ as common subjects, ‘chemistry’ as general elective subjects, and the ‘material and energy’, ‘world of chemical reactions’ as career elective subjects. ‘integrated science' is composed of power and energy, material, life, and the earth in an integrated way and consists of 6 units: the basics of science, matter and regularity, system and interaction, change and diversity, environment and energy, and science and future society. ‘chemistry’ consists of 4 units: the first step of chemistry, the world of atoms and molecules, the properties of solutions, and chemical equilibrium and reaction rates. ‘matter and energy’ consists of 4 units: thermochemical reactions, three states of matter, chemical equilibrium, and reaction rates. ‘world of chemical reaction’ consists of 4 units: acid-base, acid-base reaction, redox reaction, and application of redox reaction.

Symposium : **EDU-2**
Current Trends in Chemistry Education
Room 301 THU 16:10
Chair: Hyun-Ju Park (Chosun University)

Characteristics of the matter domain of elementary school science course in 2022 Revised Science Curriculum

Sukjin Kang

Department of Science Education, Jeonju National University of Education, Korea

The Ministry of Education emphasized that deep learning, the connection and integration of subjects, life-related learning, and the introspection of learning process should be the key points to foster students' competencies in the new 2022 Revised Science Curriculum. In this study, the Characteristics of the matter domain of elementary school science course in 2022 Revised Science Curriculum are introduced. The characteristics of the new science curriculum are noticeable in the aspects such as core ideas, three categories of content structure (knowledge/comprehension, process/skill, value/attitude), achievement standards, and directions for teaching-learning and evaluation, Educational implication for preparing and practicing the new science curriculum are discussed.

Symposium : **EDU-3**
Current Trends in Chemistry Education
Room 301 THU 16:40
Chair: Hyun-Ju Park (Chosun University)

2022 Revised Science(Chemistry) Curriculum High School Elective Course

Hyunjung Kim

Department of Chemistry Education, Kongju National University, Korea

The purpose of this presentation is to share the content elements and draft achievement standards of the high school chemistry elective course in the 2022 revised science curriculum and to hear opinions. In the 2022 revised curriculum, which will be revised along with the full implementation of the high school credit system, all subjects in high school are organized on a semester basis. ChemistryI in the 2015 revised science curriculum is opened as a general elective subject under the name of Chemistry, and the subject corresponding to ChemistryII is divided into two elective courses. The subjects corresponding to ChemistryII are selected by students in consideration of career orientation, and are opened under the names of “Material and Energy” and “The World of Chemical Reaction.” In addition, under the name of convergence choice, there are three subjects with the characteristics of climate crisis, ecological transformation, and convergence science inquiry in the big data era. At the symposium, we would like to share and hear opinions from the content elements and draft achievement standards of the three subjects, which are general electives and career electives in Chemistry. After taking Integrated Science 1 and 2, the chemistry subject to be selected in the second year of high school consists of four areas: “First Steps in Chemistry, the World of Atoms and Molecules, Properties of Solutions, Chemical Equilibrium and Reaction Rate.” It is composed of the characteristics of integrating contents corresponding to chemistry1 and 2 while weakening the level. In the case of “Material and Energy” a career elective subject, the draft was composed of four areas: “thermochemical reaction, three states of matter, chemical equilibrium, and reaction rate.” The case of “The World of Chemical Reaction” was composed of the fields of “Acid-Base, Acid-Base Reaction, Redox Reaction, and Application of Redox Reaction.” The achievement standards will be revised after collecting opinions from academic societies and field schools.

Symposium : **EDU-4**
Current Trends in Chemistry Education
Room 301 THU 17:10
Chair: Hyun-Ju Park (Chosun University)

Tailored Edutech based SDL(Self directed Learning) for highschool R&E

Eun-Young Choi

Chemistry & Biology, Korea Science Academy of KAIST, Korea

For gifted high school students, many educational curricula through research, such as R&E, creative design, and graduation research, are being conducted and such R&E (Research & Education) is spreading to general high schools. Compared with general subject classes, through R&E education, students are more effective in developing comprehensive thinking skills, communication skills, critical thinking skills, problem solving skills, and research performance skills. This is because research involves not only learning knowledge, but also various activities such as problem-taking and solving, conducting research, analyzing research results, communicating, presenting, and writing thesis. The educational gap between students is getting bigger and bigger,and individual differences according to the student's educational environment are difficult factors for effective student guidance. In particular, the gap between students' research experience and knowledge is very large, making it difficult to lead students to conduct research effectively. To provide a quality education to these students, tailored Edutech-based Self-Directed Learning (SDL) is more required. Students do not need to have all the knowledge to do research. A webpage (such as google sites) with arranged video links is provided so students can self-study the relevant knowledge or skills whenever and wherever they need them. It allows students to choose the amount of learning they need to learn and the content they want to learn according to their abilities. In the beginning, teachers should invest time and effort to utilize edutech and produce necessary educational videos (eg, how to use the program, how to use analysis equipment, knowledge, etc.). If teachers are short on time, it is also helpful to find suitable learning videos. The more these materials, the more customized education is possible for students. This video is loaded on the platform, and the loaded video link is arranged in google sites, google classroom, or webpage, etc. At this time, a roadmap for each student can be configured. Students can perform self-directed learning by looking for and referring videos that are suitable for them when needed. Teachers can invest more time advising and discuss with students by saving time with providing edu-video instead of repeatedly teaching

them simple knowledge and skills. A tailored video utilizing edutech and a systematic edutech roadmap greatly help students to conduct self-directed research, creating excellent results.

Symposium : **ENVR-1**
Current Trends in Air-pollution Control Technologies
Room 202 THU 15:40
Chair: Dongwook Kim (Korea Military Academy)

Surface water effects for photocatalytic removal of volatile organic compounds

Wooyul Kim

Department of Energy Engineering, Korea Institute of Energy Technology (KENTECH), Korea

Volatile organic compounds (VOCs) has affected many air pollution problems, especially, it is toxic for indoor air quality even at small concentrations and is known as a precursor to particulate matter. Therefore, photocatalysis technology has been extensively applied with the development of LED technology for the efficient treatment of (VOCs). TiO2 has been investigated as the primary photocatalyst for removing (VOCs) with economic benefits and sufficient oxidation power. But, the problem of deactivation of the catalysts remains an unsolved problem. The degree of deactivation depends on the structure of (VOCs)). In this work, the chain-type structure of acetaldehyde (C2H4O) and ring-type toluene (C7H8) were selected to explain the difference as representative materials. Also, the effect of atmospheric humidity on catalytic activity was observed. It is related to the removal efficiency of both substances and has a particular influence on the mineralization of toluene. In this research, we investigated the relationship between the photodegradation behavior of the (VOCs) and atmospheric humidity based on real-time Fourier transform-infrared (FTIR) analysis. Research of real-time changes with humidity in these (VOCs) photodegradation reactions can identify the cause of instability of catalysts, which can offer a basis to propel real-life application of photocatalytic technology for removing the harmful (VOCs) for safe air quality.

Symposium : **ENVR-2**

Current Trends in Air-pollution Control Technologies

Room 202 THU 16:10

Chair: Dongwook Kim (Korea Military Academy)

Low-temperature induced oxidative removal of VOCs over metal loaded TiO_2

Hyoung-il Kim

Civil and Environmental Engineering, Yonsei University, Korea

It is important to develop a clean and efficient method to control indoor air pollutants (e.g., volatile organic compounds (VOCs)) considering their carcinogenic and respiratory effects in human. Thermocatalysis is recognized as a promising and eco-friendly alternative to the conventional adsorption process owing to outstanding performance for VOC oxidation in the wide range of concentrations. However, the thermocatalysis for VOC degradation reported so far have been too limited to require a high reaction temperature (e.g., above 300 °C) to achieve a viable performance. To address these limitations, we herein present a novel indoor air purification strategy that utilizes the waste-heat harnessed by a lampshade coated with Pt-TiO_2 catalysts. In the proposed design, the Pt-TiO_2 coated on the lampshade successfully enabled the utilization of waste-heat from an indoor lamp and mineralization of CH_3CHO into CO_2. Particularly, this study systematically investigates the significant potential of thermocatalytic lampshade coated with Pt-TiO_2 as a promising alternative to conventional adsorption processes currently most widely used in indoor environments and demonstrates detailed catalytic mechanisms of the proposed Pt-TiO_2 based thermocatalysis at low-elevated temperature.

Symposium : **ENVR-3**

Current Trends in Air-pollution Control Technologies

Room 202 THU 16:40

Chair: Dongwook Kim (Korea Military Academy)

The efficient energy system of complex air pollution mixture abatement

Jaewon Han

R&D Center, SN co.,Ltd, Korea

It is necessary to control exhaust gases containing hydrogen chloride (HCl), sulfur oxides (SOx), and nitrogen oxides (NOx), which are the main causes of fine dust generation in power plants system. However, the existing wet and semi-dry reactor (SDR) have a problem of temperature decrease during the removal of acid gas. Thus, it requires additional heat energy for the SCR (Selective Catalytic Reduction) reaction of the downstream stage for NOx removal.To remove additional energy supply, we demonstrated the SRx (Sorbent Reaction Accelerator) based on dry reaction and the low-temperature SCR reactor in the power plant. For on-site optimization of the system, we designed a demonstration device using CFD programming and analyzed the performance of high active reactants which were used in this system. The NOx after primary removal in SNCR (Selective non-catalytic reduction) was eliminated in the low-temperature SCR without additional energy supply. As a result of the exhaust gas analysis after the demonstration, the concentration of HCl, SOx, and NOx are 3 ppm, 5 ppm, and 10 ppm, respectively. These results show to reduce fine dust causes by 30-50% compared to the existing ones and to satisfy the reinforced emission regulations.

Oral Presentation : **POLY.O-1**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 09:00

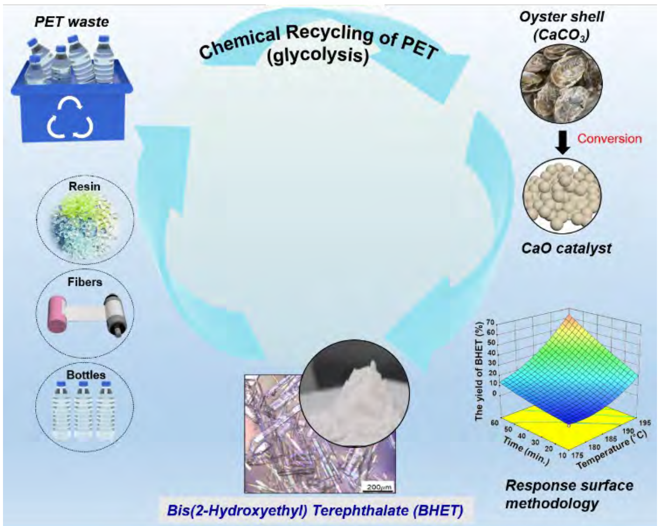
Chair: Min Sang Kwon (Seoul National University)

Optimizing PET Glycolysis with an Oyster Shell-Derived Catalyst Using Response Surface Methodology

Yonghwan Kim

Advanced Materials R&D Center, DAE-IL Corporation, Korea

Polyethylene terephthalate (PET) waste was depolymerized into bis(2-hydroxyethyl) tereph-thalate (BHET) through glycolysis with the aid of oyster shell-derived catalysts. The equilibrium yield of BHET was as high as 68.6% under the reaction conditions of mass ratios (EG to PET = 5, catalyst to PET = 0.01) at 195 °C for 1 h. Although biomass-derived Ca-based catalysts were used for PET glycolysis to obtain BHET monomers, no statistical analysis was performed to optimize the reaction conditions. Thus, in this study, we applied response surface methodology (RSM) based on three-factor Box–Behnken design (BBD) to investigate the optimal conditions for glycolysis by analyzing the independent and interactive effects of the factors, respectively. Three independent factors of interest include reaction time, temperature, and mass ratio of catalyst to PET under a fixed amount of ethylene glycol (mass ratio of EG to PET = 5) due to the saturation of the yield above the mass ratio. The quadratic regression equation was calculated for predicting the yield of BHET, which was in good agreement with the experimental data (R2 = 0.989). The contour and response surface plots showed the interaction effect between three variables and the BHET yield with the maximum average yield of monomer (64.98%) under reaction conditions of 1 wt% of mass ratio (catalyst to PET), 195 °C, and 45 min. Both the experimental results and the analysis of the response surfaces revealed that the interaction effects of reaction temperature vs. time and temperature vs. mass ratio of the catalyst to the PET were more prominent in comparison to reaction time vs. mass ratio of the catalyst to the PET.


PET waste
Chemical Recycling of PET
(glycolysis)
Oyster shell
($CaCO_3$)
Conversion
CaO catalyst
Resin
Fibers
Bottles
The yield of BHET (%)
70
60
50
40
30
20
10
0
60
50
40
30
20
10
Time (min.)
175
180
185
190
195
Temperature (°C)
200μm
Response surface
methodology
Bis(2-Hydroxyethyl) Terephthalate (BHET)

Oral Presentation : **POLY.O-2**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 09:10

Chair: Min Sang Kwon (Seoul National University)

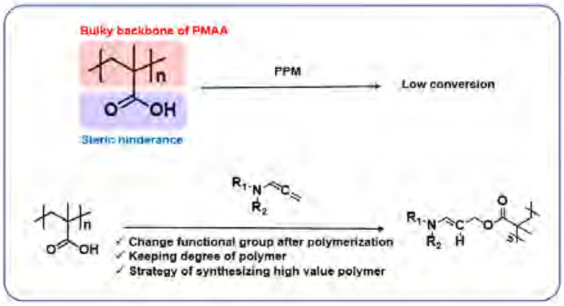
The esterification of PMAA (Poly methyl methacrylate) with allene amide via post-polymerization modification

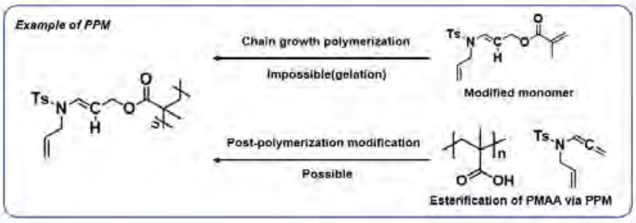
Hyungyu Shin, Jeung Gon Kim[1,*]

chemistry department, Jeonbuk National University, Korea

[1]*Department of Chemistry, Jeonbuk National University, Korea*

Post-polymerization modification (PPM) is useful method modifying the functional group of polymer after polymerization. Although general method is that polymer is synthesized by modified monomer before polymerization, using PPM can give many advantages in synthesis of polymer. PPM is well-known as a strong approach for synthesizing high-value polymers. This tool can overcome direct polymerization's drawbacks, such as the use of costly or unstable monomers. Because PPM can directly functionlize functioanal group of the polymer, this way can keep the chain of starting polymer. PPM of the various polymers have been evaluated excluded poly (methyl methacrylic acid) (PMAA) esterification due to acid functional group of PMAA being sterically hindered because of CH3 backbone. Allene amide is widely used functional group for various reactions such as coupling and heterocyclic reaction in organic chemistry. A combination of carboxylic acid and allene amide was achieved with highly chemo-selective (E-selectivity) and gave excellent yields (Park et al.). In this study, we focused on PMAA as bulky and sterically hindered carboxylic acid. Without any metal catalyst or pH control, the reaction between allene amide and PMAA showed an outstanding conversion. We suggest that the result is promising strategy for further modification of PMAA.


Bulky backbone of PMAA
n
O
OH
Steric hinderance
PPM
Low conversion
R1
N
R2
n
O
OH
✓ Change functional group after polymerization
✓ Keeping degree of polymer
✓ Strategy of synthesizing high value polymer
R1
N
R2
C
H
O
O


Example of PPM
Chain growth polymerization
Impossible(gelation)
Ts
N
C
H
O
O
Modified monomer
Ts
N
C
H
O
O
Post-polymerization modification
Possible
n
O
OH
Ts
N
C
Esterification of PMAA via PPM

Oral Presentation : **POLY.O-3**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 09:20

Chair: Min Sang Kwon (Seoul National University)

Universal Suzuki−Miyaura Catalyst-Transfer Polymerization Using Buchwald Pd G3 Precatalysts for Precision Synthesis of Strong Donor/Acceptor-Based Conjugated (Co)polymers

Jaeho Lee, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

Living catalyst-transfer polymerization has revolutionized the field of polymer synthesis, but for a given catalyst system, the polymer scope is rather narrow. Herein we report a highly efficient Suzuki−Miyaura catalyst-transfer polymerization (SCTP) of various donor (D) and acceptor (A) (hetero)arene monomers such as 3,4-propylenedioxythiophene (ProDOT), benzotriazole (BTz), quinoxaline (QX), and 2,3-diphenylquinoxaline (QXPh), by using rationally designed boronates and commercially available Buchwald precatalysts. As a result, PProDOT, PBTz, PQX, and PQXPh were prepared with controlled molecular weight and narrow dispersity in excellent yield. Structural analysis of the polymer by ^{1}H NMR and MALDI-TOF spectrometry supported the chain-growth mechanism and the high initiation efficiency of the SCTP method. In addition, the excellent catalyst-transfer ability of RuPhos−Pd led to unprecedented controlled D−A statistical copolymerization, thereby affording copolymers with tailored HOMO energy level and band gap energy. Moreover, various combinations of D−A and A−A block copolymers were successfully prepared, highlighting the living nature of SCTP. Finally, simple but powerful one-shot D−A block copolymerization was achieved by maximizing the propagating rate difference between donor and acceptor monomers to afford well-defined poly(3-hexylthiophene)-*b*-poly(benzotriazole).

Oral Presentation : **POLY.O-4**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 09:30

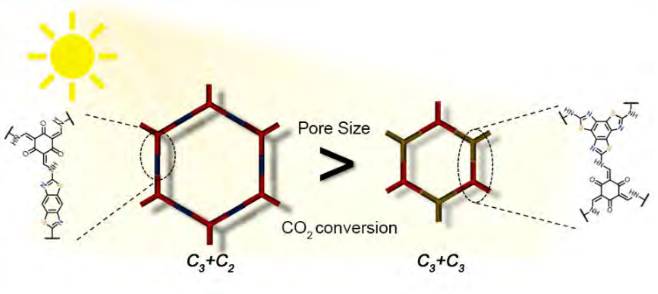
Chair: Min Sang Kwon (Seoul National University)

Tunning Porosity of Benzothiazole Based Covalent Organic Frameworks for Photocatalytic CO_2 Conversion

YoungHyun Kim, Jong-Beom Baek*

Division of Energy Engineering, Ulsan National Institute of Science and Technology, Korea

The intrinsic physical and photochemical properties of covalent organic frameworks (COFs) can be tuned by their structural features such as chemical composition of building units, linkages and their porous character. The combination of building units with different intrinsic properties can also influence their intrinsic electronic, adsorption, and optical properties. We synthesized benzothiazole-based COFs with two different combinations, composed of tris-benzothiazole triamine or bis-benzothiazole diamine with triformylphloroglucinol respectively. For their C3+C3 and C3+C2 symmetries, the hexagonal pore shaped COFs, synthesized from benzothiazole core units with approximately twice the difference in their pore size, showed good affinity with CO2 and light-harvesting properties. The COFs were then applied as photosensitizers in a photocatalytic CO2 conversion system and the larger-pore-sized COF showed a higher CO2 conversion due to the higher photocatalytic driving force stemming from proper band alignment, wider band gap, efficient charge separation and higher charge carrier mobility.



129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Oral Presentation : **POLY.O-5**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 09:40

Chair: Min Sang Kwon (Seoul National University)

NO2-Affinitive Conjugated Polymer through Side-Chain Engineering for Detection Sub-Parts-Per-Billion NO2 in Organic Field-Effect Transistor Sensor.

Yeongkwon Kang, Bong Gi Kim[1,*]

화학공학부, Konkuk University, Korea

[1]*Division of Chemical Engineering, Konkuk University, Korea*

The modification of conjugated polymer (CP) through side-chain engineering exhibited NO2-affinitive morphology and showed an exceptionally high sensitivity of 13.8 %/ppb upon NO2 (100 ppb) exposure for 50 s, and the theoretic limit of detection (LOD) reached down to 0.24 ppb with excellent selectivity toward other environmentally abundant harmful gases, such as SO2, CO2, and NH3. In particular, the LOD estimated from the CP-based field-effect transistor (FET) sensor is the lowest one for FET-based NO2 gas sensors reported until now. Morphological and structural characterizations revealed that the flexible glycol side chain enhances NO2 affinity as well as prevents the formation of lamellar stacking of the CP chains, thereby providing routes for the facile diffusion of NO2. Supplementary, theoretical calculations for CP-NO2 complex formation at the molecular level support preferential adsorption of NO2 to the polar glycol unit and a relatively low inter-chain transition barrier for NO2 within CP, which implies the spontaneous change of the NO2-binding site for the facile diffusion to the semiconductor–dielectric interface in FET-based sensor. The importance of NO2-affinitive morphology for developing highly sensitive and selective CP-based FET NO2 sensors is successfully demonstrated.

Oral Presentation : **POLY.O-6**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 09:50

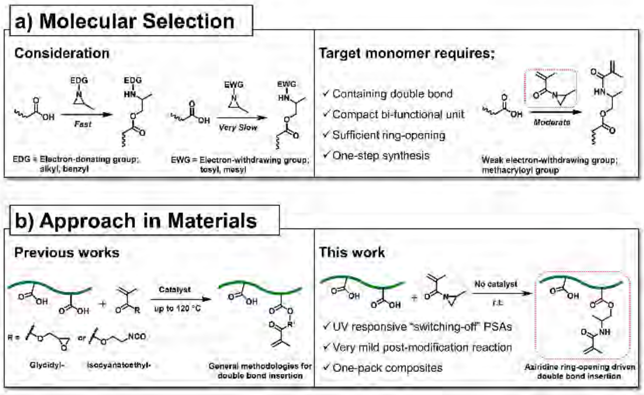
Chair: Min Sang Kwon (Seoul National University)

A facile post-modification strategy for carboxylic acid-functionalized UV-responsive pressure-sensitive adhesives

Chiwon Hwang, Hyun-jong Paik[1,*], Youngchang Yu[2,*]

Pusan National University, Korea
[1]*Department of Polymer Engineering, Pusan National University, Korea*
[2]*Center for Advanced Specialty Chemicals, Korea Research Institute of Chemical Technology, Korea*

UV-responsive pressure-sensitive adhesives (PSAs) were achieved through the ring-opening reactions of N-carbonyl aziridine radicals. By exploiting the variable ring-opening rate (depending on the N-substituent in the aziridine ring) of a suitable monomer (N-methacryloyl-2-methylaziridine), the post-modification of the carboxylic acid-functionalized acrylic PSAs was accomplished under mild conditions.The double-bond-added PSAs were characterized by spectroscopic analysis (i.e., 1H NMR and FT-IR) and their adhesion performance was evaluated under UV light irradiation (i.e., 180° peel test and loop tack test), which confirmed their "switching-off" capabilities and real-time viscosity properties and ensured a relatively long pot life. We believe our approach will render the transformation of UV-responsive polymeric materials a feasible task, which will benefit both academic research and mass-production industry.


a) Molecular Selection
Consideration
EDG
Fast
EWG
Very Slow
EDG = Electron-donating group; alkyl, benzyl
EWG = Electron-withdrawing group; tosyl, mesyl
Target monomer requires;
✓ Containing double bond
✓ Compact bi-functional unit
✓ Sufficient ring-opening
✓ One-step synthesis
Moderate
Weak electron-withdrawing group; methacryloyl group
b) Approach in Materials
Previous works
Catalyst
up to 120 °C
Glycidyl-
Isocyanatoethyl-
General methodologies for double bond insertion
This work
No catalyst
r.t.
✓ UV responsive "switching-off" PSAs
✓ Very mild post-modification reaction
✓ One-pack composites
Aziridine ring-opening driven double bond insertion

Oral Presentation : **POLY.O-7**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 10:00

Chair: Min Sang Kwon (Seoul National University)

Carbon dioxide (CO2) Based Polymer: A Sustainable Feedstock for Production of Polymer materials

Onkar S. Nayal, Min Sang Kwon*

Department of Materials Science and Engineering, Seoul National University, Korea

More than 400 million tons of polymers are produced globally every year.1 The demand for polymers has been steadily increasing at 3-4% per annum for decades and they have become an essential part of modern life.2 Even though, all their useful and versatile material properties, polymers still face a major problem: 90% of them are produced from fossil carbon, which ends up in carbon dioxide emissions.3 The associated emissions of CO2 have resulted in a significant increase in atmospheric carbon dioxide concentrations, which are thought to be responsible for global climate change and an increase in the world's average temperature.4 Although carbon is the main core atom of polymer materials, it is impossible to design and produce carbon-free polymer materials. This daunting challenge can be overcome by finding alternative carbon sources of fossil feedstocks. In this context, abundant biomass and the recyclability of plastics are good substitutes for fossil feedstocks, and researchers have done a lot of work in this area.5 However, as the use of biomass and the recycling of plastics alone, will not suffice to reduce the atmospheric carbon dioxide concentration, direct and indirect CO2 mitigation could be the solution to meet the demand for virgin polymers in the future.6 Covestro, Bayer, Asahi Kasei, enabling materials, and other industries have done tremendous work on the direct and indirect carbon dioxide utilization for the synthesis of polycarbonate, polyol, polyurethane, and other polymer materials. Despite this arduous work, increasing the carbon dioxide content in polymeric materials and the development of mild and sustainable approaches are formidable challenges. Therefore, herein, the present work provides a catalyst-free, eco-friendly, and practical nucleophilic ring-opening strategy for the synthesis of carbamates through the mitigation of CO2 in water at ambient temperature and further their utilization in the synthesis of polymer materials. This ring-opening reaction is highly efficient and practical since it works under metal-free, neutral, aqueous media and at room temperature in which the products even can be obtained by simple filtration without the need for column chromatography. The developed strategy also shows excellent compatibility with various amino acids, amines, hydrazine, hydrazides and provides excellent yields of respective carbamates.

Oral Presentation : **POLY.O-8**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 10:10

Chair: Min Sang Kwon (Seoul National University)

"Quarantined" Ring-Expansion Metathesis Polymerization: Efficient preparation of pure cyclic polymers

Jinkyung Noh, Ki-Young Yoon[1], Robert H. Grubbs[1,*], Tae-Lim Choi[2,*]

Department of Chemistry, Seoul National University, Korea
[1]*Division of Chemistry and Chemical Engineering, California Institute of Technology, United States*
[2]*Division of Chemistry, Seoul National University, Korea*

Cyclic polymers have attracted much attention due to their distinct physical properties originating from their endless cyclic topology. However, scalable preparation of pure cyclic polymers using metathesis polymerization was still limited due to the catalyst's vulnerability and inseparability. Herein, we designed an effective cyclic polymer preparation process where polymerization – polymer separation – catalyst recovery steps occur in situ. In this circular system, the pure cyclic polymer was easily dispensed after bulk ring-expansion metathesis polymerization of cyclopentene. This straightforward process was enabled by silica-supported ruthenium metathesis catalysts and customized glassware which can quarantine the catalysts from the reaction and enable efficient polymer segregation.

Oral Presentation : **POLY.O-9**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 10:20

Chair: Min Sang Kwon (Seoul National University)

Novel Acetal Group Incorporated Indacenodithiophene(IDT): Enhancement of Thermoelectricity and Conductivity via Directing position on Dopant

JInhwan Byeon, Sukwon Hong*

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Novel acetal derivatives of indacenodithiophene (IDT) were developed. Because of its high charge carrier mobility in the amorphous state, conductive polymers containing IDT units have been potential candidates for high thermoelectric performance materials. Despite this, IDT-containing polymers usually have low conductivity. Herein, we report that the insertion of unique acetal moeity into the IDT unit improves the conductivity and thermoelectric performance of the IDT-containing polymer via the directing position on the dopant. The result also suggest that the low conductivity of IDT-containing polymers is thought to be caused by the non-polar side chain, which makes the polymer-dopant complex unfavorable for charge conduction.

Oral Presentation : **POLY.O-10**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 10:30

Chair: Min Sang Kwon (Seoul National University)

Synthesis of Anion-Exchange Nanoporous Membranes with Control over Pore Size and Functional Group Density

Jinyeong Oh, Myungeun Seo[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Anion exchange membrane fuel cells (AEMFCs) have recently acquired a considerable interest in the fuel cell research community. AEMFCs have advantages over the conventional proton-exchange membrane fuel cells as fast redox kinetics can be achieved using a non-precious and relatively inexpensive metal catalyst. However, suitable membrane materials for AEMFC have yet to be developed that satisfy chemical stability, high conductivity, and permselectivity. Here, we explored nanoporous polymer membranes carrying quaternary ammonium groups on the pore surface. We adopted the middle block approach in the polymerization-induced microphase separation process and subsequent postmodification to produce 3D continuous nanoporous channels with control of pore size and functional group density. Detailed characterization of the fabricated membranes and the transport behavior across the membranes will be presented.

Oral Presentation : **POLY.O-11**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 10:40

Chair: Min Sang Kwon (Seoul National University)

Silver sulfide nanocrystals as a biocompatible and full-spectrum photocatalyst for efficient light-driven polymerization in aqueous and ambient conditions

Min Sang Kwon*, Changhoon Yu[1]

Department of Materials Science and Engineering, Seoul National University, Korea

[1]*Material science and engineering, Seoul National University, Korea*

Because of current worldwide environmental issues, polymer synthesis is expected to be ready under eco-friendly ways. PET-RAFT polymerization without additives by sunlight is the best method for setting up the polymers of distinct designs. This can be accomplished by a photocatalyst (PC) which covers the full range of daylight for high effectiveness and has great water solubility, oxygen tolerance, and biocompatibility. We found that Ag2S nanocrystals (NCs) empower the PET-RAFT polymerization for various (meth)acrylic monomers under sunlight conditions. Surprisingly, "oxygen acceleration" effect is observed over Ag2S NCs-intervened polymerizations. Quantum chemical calculation joined that the radical anion intermediates are significant for the noticed uncommon practices. PET-RAFT polymerizations with Ag2S NCs could be accomplished in the biorelevant media under normal daylight illuminations, demonstrating the biocompatibility and effectiveness of the framework.

Oral Presentation : **POLY.O-12**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 10:50

Chair: Min Sang Kwon (Seoul National University)

Mechanochemical Transformation of Aziridine into Imine in Polymers

Hyo Jae Yoon*, Sangmin Jung

Department of Chemistry, Korea University, Korea

We here show that cis-N-phthalimidoaziridine moiety incorporated into a macromolecular backbone undergoes structural transformation into imine via mechanical force-induced 1,2-migration of N-phthalimido group. Notably, the migration occurs under mechanochemical condition and not thermal one. The imine is further hydrolyzed in the presence of water under ambient conditions, bifurcating into amine and aldehyde. These structural transformations are confirmed by 1H NMR and FT-IR spectroscopic analyses. Computational simulations reveal that the applied force increases the charge unbalance between the aziridine carbon and the nitrogen of phthalimido moiety and activates the N-N bond whose axis is orthogonal to the force direction. This explains the mechanism of force-induced 1,2-migration. The substrate scope of our reaction is further evaluated by calculating Fmax (the force needed for maximal deformation of mechanophore before the scission of covalent bond). Values of Fmax for N-phthalimidoaziridine derivatives formed on widely used synthetic olefinic polymers such as polybutadiene (PB), polyacetylene (PA), polyisoprene (PI), polychloroprene (PC), and diphenyl polyene (DP) fall into the Fmax range of mechanochemical 2π electrocyclic ring opening (≤ 5.7 nN). To prove this experimentally, cis-PB is post-modified to have N-phthalimidoaziridine, and force-induced transformation into the corresponding imine is observed.

Oral Presentation : **POLY.O-13**

Oral Presentation for Young Polymer Scientists

Samda Hall THU 11:00

Chair: Min Sang Kwon (Seoul National University)

Reactive Molecular Network Sol as a Building Block for Facile Synthesis of Continuous Nanoporous Membranes

Wangsuk Oh, Ji-Woong Park*

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea

Robust and pore-size-tunable nanoporous membrane are necessary for precise nanoscale filtration and membrane-facilitated chemical reaction in organic solvent medium. We recently reported urea-based reactive molecular network, which maintained dispersed state for a long period time, enabling further polymerization in the presence of additives. Phase separation of the mixture produces continuous bicontinuous blend morphology at appropriate conditions, which can be transformed into a robust nanoporous structure. Here, we introduce our findings that various polymers and organosilanes can function as phase separation inducers and porogens to obtain a continuous nanoporous membrane. The morphology and pore size distribution of the nanoporous membranes were controlled within meso-/macroporous regime by changing the fraction of the porogens. We demonstrated filtration of sub-10 nm solutes through the nanoporous membrane in addition to its long-term and chemical stability against organic solvents. The structure-forming process was critically affected by the interplay of phase separation, gelation, and evaporation of solvent and organosilane.

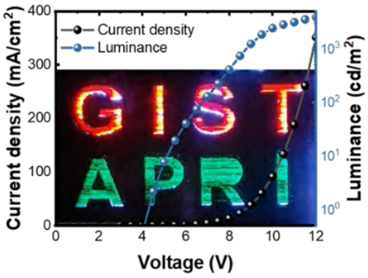
Oral Presentation : **INOR.O-1**
Oral Presentation of Young Scholars in Inorganic Chemistry
Tamna Hall B THU 09:00
Chair: Dae Woon Lim (Yonsei University)

Study on the degradation process of perovskite quantum dots to develop stable optoelectronic devices

Hanleem Lee

Chemistry, Myungji University, Korea

The perovskite quantum dots (QDs) have been great attention for a decade because of their excellent efficiency, color purity, and cost-effective fabrication. However, fast degradation (chemical, environmental, thermal, and electrical instability) of perovskite QD film leads unsuccess of establishing multi-color patterning technology, and it becomes a major obstacle to realizing high-resolution optoelectronics using this material. Therefore, the realization of high-resolution patterning is currently essential for enabling the use of perovskite QDs for next-generation optoelectronic devices. Previously, the patterned LEDs with these materials are nearly impossible to fabricate in ambient condition unlike other type of colloidal QDs. To realize patterned LEDs, the perovskite QD layer should be thin enough to facilitate the carrier injection, but it should exhibit high chemical stability with outstanding photo-physical properties.In this study, we investigate the degradation mechanism of perovskite QDs, and consider that the kinetic of surface ligands[1] and cation migration[2] played a critical role in the degradation of perovskite QDs. To prevent the degradation process of perovskite QDs, ultrathin shell coating[3] and UV cross-linkable ligand system have been developed. Due to the slow dissociation of the bound ligand in our novel UV cross-linkable ligand system, the PLQY of perovskite QDs increases by ~18% after introduction of newly developed ligand system, and its chemical stability is also drastically improved. As a result, the EL device with high resolution (~ 1 um line array) is obtained via inkjet printing. The outstanding controllability of the perovskite QDs ink facilitates the fabrication of microsize pattern perovskite quantum dot LEDs (PeLEDs) with high luminescence using red and green perovskite QDs.[1][1] H. Lee et al., Advanced Materials, 2007855, 2021[2] H. Lee et al., Nanoscale, 2022 (online publication).[3] C. K. Trinh‡, H. Lee‡, M. G. So, C-L Lee, ACS Applied Materials and Interfaces, 13, 25, 2021.


Current density
Luminance
Current density (mA/cm^2)
Luminance (cd/m^2)
Voltage (V)
0
100
200
300
400
0
2
4
6
8
10
12
10^0
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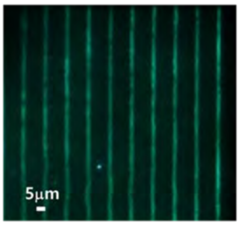
10^2
10^3
GIST
APRI


5μm

Oral Presentation : **INOR.O-2**

Oral Presentation of Young Scholars in Inorganic Chemistry

Tamna Hall B THU 09:20

Chair: Dae Woon Lim (Yonsei University)

Magnetic ordering through itinerant ferromagnetism in a metal–organic framework

Jesse Gaehyun Park

Chemistry, Korea Advanced Institute of Science and Technology, Korea

Materials that combine magnetic order with other desirable physical attributes could find transformative applications in spintronics, quantum sensing, low-density magnets and gas separations. Among potential multifunctional magnetic materials, metal–organic frameworks, in particular, bear structures that offer intrinsic porosity, vast chemical and structural programmability, and the tunability of electronic properties. Nevertheless, magnetic order within metal–organic frameworks has generally been limited to low temperatures, owing largely to challenges in creating a strong magnetic exchange. Here we employ the phenomenon of itinerant ferromagnetism to realize magnetic ordering at $T_C = 225$ K in a mixed-valence chromium(II/III) triazolate compound, which represents the highest ferromagnetic ordering temperature yet observed in a metal–organic framework. The itinerant ferromagnetism proceeds through a double-exchange mechanism, which results in a barrierless charge transport below the Curie temperature and a large negative magnetoresistance of 23% at 5 K. These observations suggest applications for double-exchange-based coordination solids in the emergent fields of magnetoelectrics and spintronics.

Oral Presentation : **INOR.O-3**

Oral Presentation of Young Scholars in Inorganic Chemistry

Tamna Hall B THU 09:40

Chair: Dae Woon Lim (Yonsei University)

Development of unconventional hetero nanostructures with metastability

Jongsik Park

Department of Chemistry, Kyonggi University, Korea

The success of water electrolysis is critically dependent on the performance of electrocatalysts in both half-cell reactions of oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), thus calling for the design of active yet durable catalyst surface and for the prudent choice of catalyst material phase. The recent advances in this field show that the introduction of metastable nanocrystals can greatly modify the surface energy of the catalyst. From this point of view, the post-synthetic transformation of nanoparticles such as cation exchange reaction has received great attention, because this approach can provide an unusual route to elaborately composition-controlled nanostructures while maintaining the overall structure of the template. Herein, we demonstrate that the development of nanocrystals having metastable phase could be achieved through the choice of rationally designed nano template via the post-modification method. We expect that the unique composition fluctuations in multiphasic nanostructures with metastable phases will provide new synthetic methodologies for the design and synthesis of intricate nanostructures with novel physicochemical properties.

Oral Presentation : **INOR.O-4**

Oral Presentation of Young Scholars in Inorganic Chemistry

Tamna Hall B THU 10:00

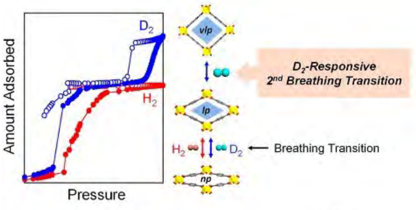
Chair: Junsang Cho (Sungshin University)

Novel MOF-based Systems for Molecular Recognitions

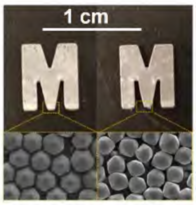
Jin Yeong Kim, Hyunchul Oh[1,*], Hoi Ri Moon[2,*]

Department of Chemistry Education, Seoul National University, Korea
[1]*Department of Energy Engineering, Gyeongsang National University, Korea*
[2]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Metal-organic Frameworks(MOFs) are crystalline porous materials with high structural and functional tunability and have been explored as next-generation selective molecular recognition sorbents for the separation of challenging mixtures. In this presentation, two novel MOF-based systems for molecular recognition are introduced. One is a unique isotope-responsive flexible MOF, MIL-53(Al), which can selectively recognize and respond to only D_2 molecules through a secondary breathing transition. The other is a simple but novel strategy proposed which exploits directional anisotropy in MOFs to modulate the characteristics of MOFs. A one-step strategy to control the 2D assembly of nanoporous polyhedral MOF crystals through simple changes in the casting solvent and subsequent immobilization of these oriented particles in large area polymer films is reported. Our works can serve as a starting point to accelerate the discovery of novel MOF-based systems that can potentially be used for the purification of challenging mixtures.



Specific isotope-responsive MOF



Aligned MOF film

Oral Presentation : **INOR.O-5**

Oral Presentation of Young Scholars in Inorganic Chemistry

Tamna Hall B THU 10:20

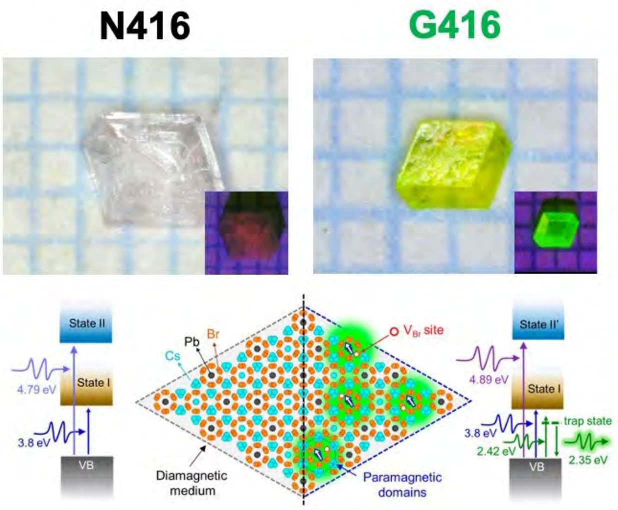
Chair: Junsang Cho (Sungshin University)

Superparamagnetism and Photoluminescence of Zero-Dimensional Cs_4PbBr_4 Perovskite Crystals

Ji-Hyun Cha

Department of Chemistry, Chungnam National University, Korea

Inorganic halide perovskites have attracted considerable attention as promising materials for optoelectronic applications. The outstanding optoelectrical properties of halide perovskite materials are closely related to their crystal structures. Zero-dimensional (0D) inorganic halide perovskites with a stoichiometry of Cs_4PbBr_4 have been heavily investigated due to their robust photoluminescence (PL) properties. However, the origin of the unusual green emission in Cs_4PbBr_4 remains an open question. To understand the strong green emission from 0D Cs_4PbBr_4 perovskites, we prepared Cs_4PbBr_4 single crystals with and without green emission for comparing their structural, magnetic, and optical properties. We revealed that non-emissive Cs_4PbBr_4 (N416) crystal exhibits exclusive diamagnetic properties, while green Cs_4PbBr_4 (G416) crystal possesses both diamagnetic and paramagnetic components, demonstrating the existence of paramagnetic electron spins in the G416 crystal induced by crystal defects. The lattice contraction, Cs atomic charge change, and electronic state shift are observed by comparing synthesized G416 and N416, and their simulation results using the Br vacancy model agree with these experimental observations. This observation allows us to correlate the green PL of the G416 crystal to the presence of Br vacancies, which probably plays a role as a paramagnetic domain and green emission center.


N416
G416
State II
4.79 eV
State I
3.8 eV
VB
Pb
Br
Cs
Diamagnetic medium
V_{Br} site
Paramagnetic domains
State II'
4.89 eV
State I
3.8 eV
2.42 eV
trap state
2.35 eV
VB

Oral Presentation : **INOR.O-6**

Oral Presentation of Young Scholars in Inorganic Chemistry

Tamna Hall B THU 10:40

Chair: Junsang Cho (Sungshin University)

Effective Softness-Driven Self-Assembly Behavior of Polymer-Coated Nanocrystals

Hongseok Yun

Department of Chemistry, Hanyang University, Korea

Colloidal inorganic nanocrystals (NCs) are attractive building blocks for designing novel metamaterials with complicated structures. Since the properties of NCs depend not only on the morphology of individual NCs but also on their assembled packing symmetries, it is highly important to understand the self-assembly behavior of NCs. Herein, we present precise control of self-assembled superlattice symmetry of polystyrene-coated Au (Au@PS) nanoparticles (NPs) by changing their core size, ligand length, and grafting density. Au@PS NPs were synthesized through ligand exchange using thiol-terminated PS with different molecular weights (Mn). The Au@PS NPs were then self-assembled through liquid-air interface self-assembly process. Transmission electron microscopy images and grazing incidence small-angle X-ray scattering data showed well-ordered Au@PS superlattices. In particular, symmetry transitions from hexagonal close packing (hcp) to body-centered cubic (bcc) symmetry were found as either Mn increases or NC diameter decreases. To explain these phenomena, we proposed an “effective softness” model, considering concentrated polymer brushes (CPB) around NC surface as part of “hard core.” Finally, the interparticle distance of polymer-grafted NCs was theoretically calculated based on the combination of the optimal packing model (OPM) and the effective softness model.

Oral Presentation : **PHYS.O-1**

Oral Presentation for Young Physical Chemists

Halla Hall THU 09:00

Chair: Jooyoung Sung (DGIST)

Dynamic Stark Effect on Non-valence Bound States of Polyatomic Molecular Anions

Do Hyung Kang, Jinwoo Kim, Sang Kyu Kim*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Quasi-free electron bound in atoms or molecules often plays a role of key initiator in various chemical reactions. Manipulating the bound character of excess electron may provide dynamic control of subsequent reaction rate or pathway, yet it is still in its infancy on the polyatomic molecular systems. Herein, we present the experimental observation of the dynamic Stark effect on non-valence bound states (NBS) of polyatomic molecular anions by exploiting the strong picosecond laser pulse. As the non-valence electron is weakly bound in neutral core by long-range potentials (charge-dipole or charge-quadrupole interaction), excess electron in NBS exhibits the ponderomotive blue-shift induced by the external oscillating electromagnetic field. Quasi-free quadrupole-bound electron is found to be more susceptible with respect to the laser field compared to the dipole-bound electron, implying the diffuse and more polarizable nature of quadrupole-bound state (QBS) compared to the dipole-bound state (DBS). This finding promises the quantum manipulation of polyatomic systems by employing the ponderomotive effect induced by oscillating laser field in the near future.[1] D. H. Kang, S. An and S. K. Kim, Phys. Rev. Lett. 125, 093001 (2020).[2] D. H. Kang, J. Kim, M. Cheng and S. K. Kim, J. Phys. Chem. Lett. 2021, 12, 1947-1954.[3] D. H. Kang, J. Kim, H. R. Noh and S. K. Kim, Nat. Commun. 12, 7098 (2021).

Oral Presentation : **PHYS.O-2**

Oral Presentation for Young Physical Chemists

Halla Hall THU 09:10

Chair: Jooyoung Sung (DGIST)

Time-Resolved Cathodoluminescence of Nanodiamond Color Centers in Ultrafast Electron Microscopy

Ye-Jin Kim, Oh-Hoon Kwon*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

The modern technologies of light-emitting devices, light harvesting, and quantum information processing requires understanding of structure-function relations at spatial scales below the optical diffraction limit and the timescales of energy and information flows [1]. Here, we uniquely combine cathodoluminescence (CL) with ultrafast electron microscopy (UEM) [2-4]. A synergistic use of the two methodologies is essential because CL and UEM pose with required spectral and spatiotemporal sensitivity, respectively [4,5]. For color centers in nanodiamonds, we demonstrate the measurement of CL lifetime with the local sensitivity of 50 nm and the time resolution of 100 ps. It is revealed that the emitting states of the color centers can be populated by charge transfer among the color centers across diamond lattices upon high-energy electron beam excitation. The technical advance achieved in this study will deliver new concepts for specific control over energy conversion at nanoscales relevant to quantum dots and single-photon sources.[1] Nayak, P. K. et al., Nat. Rev. Mater. 2019, 4, 269-285.[2] Kim, Y.-J. et al., Matter 2019, 1, 481-495.[3] Kim, Y.-J. et al., ACS Nano 2020, 14, 11383-11393.[4] Kim, Y.-J. and Kwon, O.-H., ACS Nano 2021, 15, 19480-19489.[5] Meuret, S. et al., Appl. Phys. Lett. 2021, 119, 062106.

Oral Presentation : **PHYS.O-3**

Oral Presentation for Young Physical Chemists

Halla Hall THU 09:20

Chair: Jooyoung Sung (DGIST)

Structural dynamics of homodimeric hemoglobin in the ultrafast time domain revealed by time-resolved X-ray solution scattering

Yunbeom Lee, **Hyotcherl Ihee**[1,*]

Center for Advanced Reaction Dynamics, Institute for Basic Science, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Due to its simple dimeric structure and cooperative ligand binding, homodimeric hemoglobin (HbI) has served as a model system for the cooperative behavior of proteins [1, 2]. Still, due to the limited time resolutions of the previous studies, the ultrafast structural dynamics of HbI had remained vague. Here, we present the ultrafast structural dynamics of HbI in the solution phase revealed by femtosecond time-resolved X-ray solution scattering (fs-TRXSS) with a sub-picosecond time resolution, which was performed at an X-ray free-electron laser [3]. According to our simulation on the effect of the electron density change of the hydration shell on the fs-TRXSS data, the signal originating from the hydration shell change was dominant in the small-angle X-ray scattering (SAXS) region of the fs-TRXSS data, whereas it was not significant in the wide-angle X-ray scattering (WAXS) region. Based on this result, the structural dynamics of the bare protein were unraveled by analyzing the WAXS region. For example, we identified the formation of a reaction intermediate (I_0), which was not reported in the previous TRXSS study, and the coherent motion of HbI. In addition to the structural change of the protein, the change of the electron density of the hydration shell was unveiled by analyzing the SAXS region, based on the idea that the signal in the SAXS region is largely affected by the change of the hydration shell.[1] Proc. Natl. Acad. Sci. U. S. A., 103, 7649 (2006)[2] J. Am. Chem. Soc., 134, 7001-7008 (2012)[3] Nat. Commun., 12, 3677 (2021)

Oral Presentation : **PHYS.O-4**

Oral Presentation for Young Physical Chemists

Halla Hall THU 09:30

Chair: Jooyoung Sung (DGIST)

Strong Modulation of Nonlinear Optical Response Mediated by Interlayer Coupling in 2D Heterostructures

Gyouil Jeong, Sunmin Ryu*

Department of Chemistry, Pohang University of Science and Technology, Korea

Second-harmonic generation (SHG) is a nonlinear optical process where two photons with same energy convert into new photon with twice the energy. Transition metal dichalcogenides (TMDs) have been spotlighted due to their strong SHG efficiency and atomic thickness circumventing phase-match problem. In addition, various combinations of TMDs enables us to fabricate heterostructures with desirable nonlinear optical property. In this paper, we report that interlayer coupling dramatically affects SHG response of individual monolayer in $MoSe_2/WS_2$. We were able to exclusively monitor SHG of specific monolayer out of heterostructure using polarization-resolved detection, which revealed SHG intensity becomes remarkably different in hetero-region compared to unstack monolayer. Especially, this behavior was strengthened when photon energy matches with exciton resonance of adjacent layer. In addition, SHG phase also depended on wavelength periodically. Using hBN-inserted $MoSe_2/WS_2$, we found that this behavior disappeared in spite of ~ 2 nm distance. Based on these results, possible candidates for interlayer coupling will be discussed.

Oral Presentation : **PHYS.O-5**

Oral Presentation for Young Physical Chemists

Halla Hall THU 09:40

Chair: Jooyoung Sung (DGIST)

DNA bending affects the formation of Z-DNA investigated by single-molecule FRET

Jaehun Yi, Nam Ki Lee[1,*]

Department of Chemistry, Seoul National University, Korea
[1]*Division of Chemistry, Seoul National University, Korea*

Z-DNA, a non-canonical helical form of double stranded DNA (dsDNA), plays a pivotal role in various biological processes such as transcription regulation. In previous work, Z-DNA is formed under mechanical stress such as torsion and tension. However, the effect of bending, one of the most common deformations of DNA, on Z-DNA formation is totally unknown. In order to investigate, we modulated the bending force on dsDNA without any external forces using D-shaped DNA nanostructures. Then, we measured single-molecule fluorescence resonance energy transfer via alternating-laser excitation confocal microscopy. Herein, we show that DNA bending involves in the formation of Z-DNA. That is, the B-Z transition midpoint differs depending on the bending force. Our result provides a new insight into the effect of DNA bending on Z-DNA formation.

Oral Presentation : **PHYS.O-6**

Oral Presentation for Young Physical Chemists

Halla Hall THU 09:50

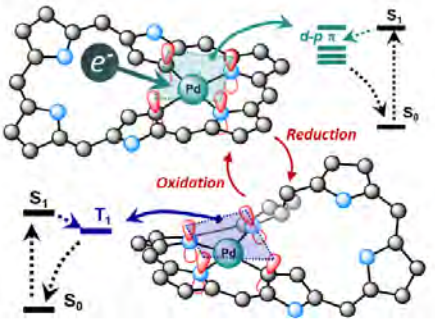
Chair: Jooyoung Sung (DGIST)

Modulations of a Metal–Ligand Interaction and Photophysical Behaviors by Hückel–Möbius Aromatic Switching

Jinseok Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

In organometallic complexes containing π-conjugated macrocyclic chelate ligands, conformational change significantly affects metal−ligand electronic interactions, hence tuning properties of the complexes. In this regard, we investigated the metal−ligand interactions in hexaphyrin mono-Pd(II) complexes Pd[28]M and Pd[26]H, which exhibit a redox-induced switching of Hückel− Möbius aromaticity and subsequent molecular conformation, and their effect on the electronic structure and photophysical behaviors. In Möbius aromatic Pd[28]M, the weak metal−ligand interaction leads to the π electronic structure of the hexaphyrin ligand remaining almost intact, which undergoes efficient intersystem crossing (ISC) assisted by the heavy-atom effect of the Pd metal. In Hückel aromatic Pd[26]H, the significant metal−ligand interaction results in ligand-to- metal charge-transfer (LMCT) in the excited-state dynamics. These contrasting metal−ligand electronic interactions have been revealed by time-resolved electronic and vibrational spectroscopies and time-dependent DFT calculations. This work indicates that the conspicuous modulation of metal−ligand interaction by Hückel−Möbius aromaticity switching is an appealing approach to manipulate molecular properties of metal complexes, further enabling the fine-tuning of metal−ligand interactions and the novel design of functional organometallic materials.


e-
Pd
d-p π
S1
S0
Reduction
Oxidation
S1
T1
Pd
S0

Oral Presentation : **PHYS.O-7**

Oral Presentation for Young Physical Chemists

Halla Hall THU 10:00

Chair: Jooyoung Sung (DGIST)

Photo-induced promotion of reductive elimination reactions of $Ni^{II/III/IV}$ complexes via C-to-Ni charge-transfer excited states

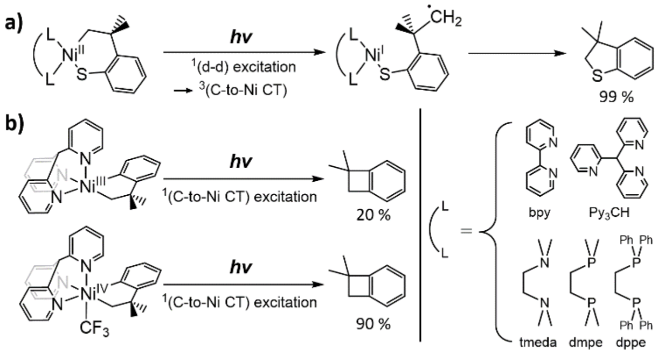
Jeongcheol Shin, Jiseon Lee, Suyeon Gwon, Samhwan Kim, Kiyoung Park*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

While photoexcitation had become one of the acknowledged methods to activate Ni-catalyzed cross-coupling reactions, factors that govern the photoactivity of organonickel complexes still have not been established. In our recent studies, we have proposed the C-to-Ni charge transfer (CT) states as key excited states for photoexcitation-induced reductive elimination (RE) reactions of nickelacycle complexes. Here I present two different examples of photo-induced RE reactions: *C-S bond-forming RE reactions of* Ni^{II} *complexes* and *C-C bond-forming RE reactions of* Ni^{III} *and* Ni^{IV} *complexes*. The excited-state C-S bond-forming RE activities of nickelacycles with the thiacycloneophyl ($-SC_6H_4$-*o*-$C(CH_3)_2CH_2-$) ligand have been investigated with five different ancillary ligands, revealing that the RE activities depend on the excitation energy and are independent of the ancillary ligand. The electronic structural analyses utilizing electronic absorption (Abs) and magnetic circular dichroism (MCD) spectroscopies in combination with density functional theory (DFT) computations have uncovered that ligand-field excitations can induce Ni-C bond homolysis via intersystem crossing to a dissociative ^{3}(C-to-Ni CT) surface, resulting in the Ni^{I} intermediate that can undergo C-S coupling. Alternatively, with cycloneophyl ($-C_6H_4$-*o*-$C(CH_3)_2CH_2-$) Ni^{III} and Ni^{IV} complexes, C-to-Ni CT excited states are directly accessible, exhibiting 10^5-time enhanced C-C bond-forming activity compared to the ground state. These studies emphasize that the RE reactions of Ni complexes can be promoted by accessing C-to-Ni CT excited states, showing the significance of understanding reaction mechanisms at an electronic structure level. Furthermore, these mechanistic elucidations provide an understanding of excited-state RE reactions of organonickel complexes, which can be utilized to design the Ni catalysts for photoexcitation-induced cross-coupling reactions.

[1]J. Shin, J. Lee, J.-M. Suh, K. Park. *Chem. Sci.* **2021**, *12*, 15908-15915.

[2]J. Shin, S. Gwon, S. Kim, J. Lee, K. Park. *J. Am. Chem. Soc.* **2020**, *142*, 4173-4183.


a)
hv
1(d-d) excitation
→ 3(C-to-Ni CT)
99 %
b)
hv
1(C-to-Ni CT) excitation
20 %
hv
1(C-to-Ni CT) excitation
90 %
L =
bpy
Py3CH
tmeda
dmpe
dppe

Oral Presentation : **PHYS.O-8**

Oral Presentation for Young Physical Chemists

Halla Hall THU 10:10

Chair: Jooyoung Sung (DGIST)

Branching ratio in photodissociation of 1-bromo-3-chlorobenzen cation

Bong Gyu Jeong, Jae Kyu Song[*], Seung Min Park[*]

Department of Chemistry, Kyung Hee University, Korea

The new method for branching ratio based on Rice-Ramsperger-Kassel-Marcus (RRKM) theory with extremely loose transition state (RRKM-eLTS) was adopted to analyze experimental results in photodissociation. The RRKM-eLTS estimated branching ratio without challenging calculation such as structure or frequencies of the transition state. We examined this method thorough comparison of experimental results that photodissociation of 1-bromo-3-chlorobenzene (3BCB) was selected for branching ratio. The photodissociation channels of 3BCB were described by 3BCB+ → Br-dissociated daughter ion (ClBz+) + Br• and 3BCB+ → Cl-dissociated daughter ion (BrBz+) + Cl•. The branching ratio was monitored by a homebuilt tandem time of flight mass spectrometer. Although there was some discrepancy in internal energy between the experimental and calculation results, the RRKM-eLTS is worth to be extended to other diverse systems considering its intuitive and simple nature.

Oral Presentation : **PHYS.O-9**

Oral Presentation for Young Physical Chemists

Halla Hall THU 10:20

Chair: Jooyoung Sung (DGIST)

Enhanced photocatalytic activity of TiO_2 by K towards acetaldehyde and NO oxidation; role of K single ion dopants and additional K-compound structures

Shufang Zhao, HuiCheol Choe, Miyeon Jeong, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

Various amounts of K were deposited on TiO_2 (P25), and the resulting structures were used as photocatalysts for acetaldehyde and NO oxidation. For acetaldehyde under dry and moderately humid conditions, a very small amount of K boosted photocatalytic activity, whereas higher K contents resulted in declined activity. Small amount of K was shown to be inserted into TiO_2 lattice, modifying structural and optical properties of TiO_2, resulting in the enhanced photocatalytic activity, whereas excessive K formed separate and less active K-compound structure on TiO_2 surface. The photocatalytic activity was gradually decreased with increasing K content for the acetaldehyde oxidation under higher humidity conditions and NO oxidation. We highlight different role of K species in TiO_2 with different structural properties, and necessity of fine adjustment of K content in K-TiO_2 depending on the reaction and conditions, to which the photocatalysts are applied.

Oral Presentation : **PHYS.O-10**

Oral Presentation for Young Physical Chemists

Halla Hall THU 10:30

Chair: Jooyoung Sung (DGIST)

Unique mechanical response of the organic ionic plastic crystal upon shear deformation that is neither elastic nor viscoelastic

Chung Bin Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystal (OIPC) is a unique class of a crystal in which orientational disorder is allowed while a long-range translational order is maintained. The rotational disorder enables OIPCs to have multiple solid phases and undergo plastic deformations upon mechanical deformations. In this work, we show by employing atomistic molecular dynamics simulations that shear facilitates a solid-solid transition and produces unique mechanical responses. We employ 1,3-dimethyl imidazolium hexafluorophosphate ([MMIM][PF6]) crystal and the step strain method to investigate mechanical response of the crystal. From our results, at low temperature and strain, [MMIM][PF6] responses to a shear deformation like either elastic or viscoelastic solid. That is, with a step strain deformation, the crystal structure does not change or only a bending event occurs such that the stress does not decay (elastic solid) from the initial stress or converges to a smaller positive value (viscoelastic solid). On the other hand, at high temperature and strain, [MMIM][PF6] changes its structure to a new crystal structure via crystal-to-crystal transition spontaneously. During the transition, ions rearrange their positions cooperatively and cations and anions are packed up layer by layer. The temporary increase of the mobility of ions decreases the stress to a negative value which is not expected in elastic or viscoelastic solid. Thanks to the crystal-to-crystal transition, ions can accomplish higher rotational disorder in the new crystal structure.

Oral Presentation : **PHYS.O-11**
Oral Presentation for Young Physical Chemists
Halla Hall THU 10:40
Chair: Jooyoung Sung (DGIST)

Insight about the Active Sites and Bonding Characteristics of Fe Single-Atom Catalysts from XPS and First-principles Modeling

Hafiz ghulam Abbas

Physical Chemistry, Korea University, Korea

X-ray photoemission (XPS) and near-edge x-ray absorption fine structure (NEXAFS) spectroscopy are useful in the interpretation of solid's structural and electronic characteristics, as well as their surfaces. The functionalization of graphene significantly tune its properties and enhanced its potential applications. In this study, we have predicted accurate absolute core electron binding energies of graphene oxide, nitrogen-doped graphene (N_4C), nitrogen and Fe functionalized graphene (FeN_4C) as well as adsorbed atomic and molecular O, CO, and H_2O molecules on FeN_4C heterogeneous catalysts by employing the first-principle framework. We found core electron binding energy as the total energy difference between two (N-1) states, one with a core hole and one with an electron removed from the highest occupied valence state, which agrees well with empirically measured reference binding energy. Adsorption energy calculation suggests that adsorbed molecules tend to bind with Fe atoms on the surface of (FeN_4C) catalyst. Charge density analysis exhibits adsorption of oxygen molecules on the FeN_4C surface changes the oxidation state of the iron (Fe) from Fe(II) to Fe(III) due to the transfer of electrons. In addition, we have been investigated the NEXAFS spectrum of the functionalized nitrogen and the oxygen atoms of adsorbed molecules on the FeN_4C surface using the transition potential method including angular dependence on the polarization direction of incident radiation corresponding to the surface plane.

Oral Presentation : **PHYS.O-12**

Oral Presentation for Young Physical Chemists

Halla Hall THU 10:50

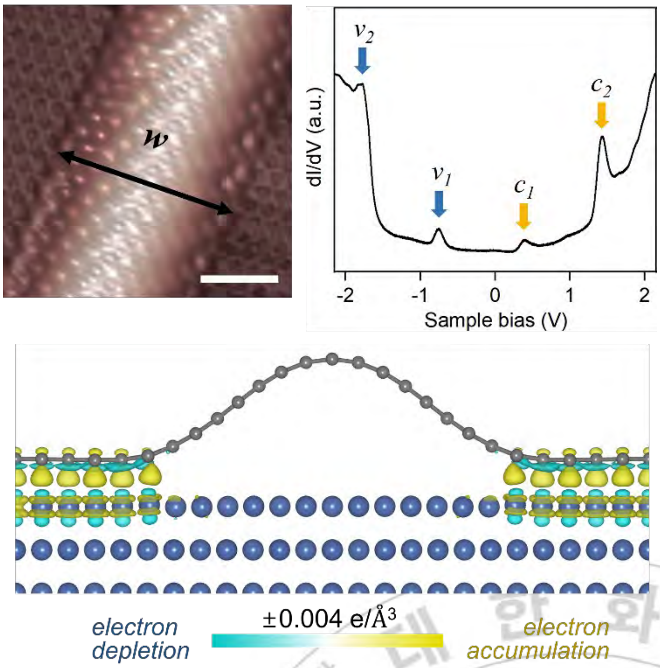
Chair: Jooyoung Sung (DGIST)

Theoretical Study of Van Hove Singularities in Graphene Nanowrinkle on Ni(111)

Jong-Guk Ahn, Hyunseob Lim[1,*], Jaehoon Jung[2,*]

Department of Chemistry, Gwangju Institute of Science and Technology (GIST), Korea
[1]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*
[2]*Department of Chemistry, University of Ulsan, Korea*

Graphene is one of the most popular two-dimensional materials. It has unique properties, such as conductivity, mechanical strength, thermal stability. Although graphene has superior conductivity, it was difficult to apply semiconductor devices because pristine graphene has no bandgap. Therefore, there are various attempts to open bandgap through chemical modification (e.g., graphene nanoribbon, graphene nanomesh). We report the van Hove singularity in graphene nanowrinkle (GNW) structure at Ni(111) surface by scanning tunnelling microscopy, it is strong evidence of quantum confinement effect. To investigate those van Hove singularities, we conducted systematic DFT calculations with GNW/Ni(111) and GNW/Cu(111). Charge difference map and orbital projected band structure revealed different interactions between graphene and each metal. Furthermore, a series of band-decomposed charge densities showed standing wave-like motion in pseudo-one dimensional confined GNW/Ni(111). Our results provide a better understanding of interfacial between graphene-metal and electronic motion at nanosized modified graphene structure.


w
v2
v1
c1
c2
dI/dV (a.u.)
-2
-1
0
1
2
Sample bias (V)
electron depletion
±0.004 e/Å3
electron accumulation

Oral Presentation : **ANAL1.O-1**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:00

Chair: Yang-Rae Kim (Kwangwoon University)

Fe-Based Mesoporous Nanostructures for Electrochemical Conversion and Storage of Energy

Lemma Teshome Tufa, Jaebeom Lee*

Chemistry, Chungnam National University, Korea

Decarbonization of the global energy system requires a coordinated effort towards disruptive technology of renewable energy conversion and storage (ECS) that can be potential to secure and diversify energy systems by increasing efficiency of conversion and storage of intermittent energy sources. Porous nanostructures have been newly reported as a promising class of most effective materials for (ECS) because of their unique advantages in terms of large surface-to-volume ratios, surface permeability, and void spaces. These offer abundant active sites for electrochemical activities by shortening the pathway of mass/charge transport. Particularly, Fe-based mesoporous nanostructures (mp-FeNSs) have been recently fascinating. Iron is a principal active center in nanocomposites and has high industrial suitability for next-generation technology owing to its environment friendliness, abundance, and low cost. Crucial technical advances related to Fe-based mesoporous nanostructures are discussed in terms of synthesis, structural design strategy, and ECS applications such as water electrocatalysis, Li-ion batteries, and supercapacitors.

Oral Presentation : **ANAL1.O-2**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:04

Chair: Yang-Rae Kim (Kwangwoon University)

Analysis of Volatile Organic Compounds Produced in Non-degradable and Biodegradable Plastics during Incineration

Min Jang, Hyemin Yang, Jeyoung Park[1,*]

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The conventional plastics undoubtedly flourished our lives and society. However, disposal of the non-degradable accumulated plastics became globally serious environmental problems. As an alternative, incineration of them are still being carried out to dispose them, but it may cause toxic volatile organic compounds (VOCs) emission. In order to solve the problems, biodegradable plastics have been developed and started to be commercialized recently. Nevertheless, biodegradable plastics are still discarded indiscreetly and mixed with the conventional non-degradable plastics due to lack of policy and limited market share, thus they can be incinerated together. Previously, studies regarding VOCs from polymers had rarely explored the level of toxicants during the combustion process. This study, for the first time, aims qualitative and quantitative analysis on VOCs emitted from both non-degradable and biodegradable plastics during combustion using gas chromatography mass spectrometry. As a result, the levels of VOCs in non-degradable poly(vinyl chloride) and poly(ethylene terephthalate) were approximately >100 times higher than biodegradable polyhydroxyalkanoate and poly(lactic acid). Interestingly, 1,3-butadiene accounts for the highest concentration among VOCs in both non-degradable and biodegradable plastics owing to the presence of butylene repeating unit. Exemplary case of gas barrier films for food packaging purpose, non-degradable aluminum-coated multi-layered film emits more of VOCs rather than biodegradable nanocellulose/nanochitin-coated film. Nevertheless, incineration of biodegradable plastics cannot be an ultimate solution because VOCs are still emitted when incompletely combusted. This study encourages the necessities of research on more diverse combustion conditions for various plastics and related discussion on the fate of discarded plastics.

Oral Presentation : **ANAL1.O-3**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:08

Chair: Yang-Rae Kim (Kwangwoon University)

Development of Raman spectroscopic scheme for non-destructive measurement of liver organoid

Sang hoon Cho, Eunjin Jang, Yunjung Kim, Hoeil Chung[*]

Department of Chemistry, Hanyang University, Korea

In the past, animal testing has been performed on living animals for purpose of assessing the possible negative effectiveness on human. However, it has been issued that problem of ethics like animal abuse and question on the necessity of animal testing when symptom only appears on human. Rather than animal testing, biomedical analysis utilizing an organoid has become an attention-drawing alternative. An organoid is cultivated from human stem cell and has similar cell composition with real organs. Therefore, toxicity test and drug reactions using organoid would be more effective than using other animals. Simultaneously, an analytical tool able to non-destructively analyze a live organoid becomes critically demanding since the destruction of organoid for analysis is not practically allowed for continuation of related toxicological and biomedical research. To meet the demand, Raman spectroscopy based on a wide area illumination (WAI) scheme providing a laser illumination diameter of 1 mm was explored. For the study, normal liver organoids (control group) were cultivated and other organoids were also prepared as non-alcoholic fatty liver (NASH) using culture medium with high fatty acid concentration. Simultaneously, to increase Raman signal of small-size organoids, a cone-shape metal-reflective cavity was prepared and the organoids with culture medium was transferred into the cavity. Then, the WAI scheme covering the whole organoids in the cavity was used to acquire corresponding Raman spectra. Raman spectral features of the control and NASH organoids were compared with each other and their differences were discussed.

Oral Presentation : **ANAL1.O-4**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:12

Chair: Yang-Rae Kim (Kwangwoon University)

Simple determination of Fe_3O_4 concentration in sintered ores by their color images

Woosuk Sohng, Seongsoo Jeong, Hoeil Chung[1,*]

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A sintered ore consists of primarily iron oxides of magnetite (Fe_3O_4) and hematite (Fe_2O_3) with other components such as CaO, SiO_2, and MgO. Since the content of Fe_3O_4 in sintered ore is necessary to determine for stable operation of the process, a titration method based on the redox reaction between Fe^2+ and $K_2Cr_2O_7$ (titrant) has been conventionally adopted; however, it is very slow and cumbersome for sample pretreatment. So, a rapid analytical method for the analysis is highly beneficial. Since the colors of Fe_3O_4 and Fe_2O_3 are black and red, respectively, the colors of sintered ores would be translated into their composition, a driving motivation for this research. With this motivation, color images (pictures) of 200 sintered ore samples with different concentrations of Fe_2O_3 were initially acquired. Then, 2 separate steps were employed to preprocess the image data. First, the difference in RGB values due to the change in brightness of illumination was calibrated (compensated) by using the 3D thin-plate spline warping (TPS-3D) with color-checker. Second, the shades or cracks and features of inorganic oxides except iron oxides were filtered through the image segmentation. Finally, using the 2 step-preprocessed image data, the corresponding Fe_3O_4 concentrations were determined using support vector regression (SVR) and resulting accuracy was comparatively discussed with that based on Raman spectroscopy. Keywords: Sintered ore; Magnetite concentration; Titration; Color image analysis; Support vector regression (SVR)

Oral Presentation : **ANAL1.O-5**
Oral Presentation of Young Analytical Chemists I
Room 201 THU 09:16
Chair: Yang-Rae Kim (Kwangwoon University)

Back-scattering based axially slanted laser illumination scheme for direct composition analysis of sample housed in a glass container

Haeseong Jeong, Sang Hoon Cho, Hoeil Chung[1,*], Daun Seol[2]

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An axially slanted illumination (ASI) scheme slantingly irradiating laser on the headspace side of a glass container and positioning a detector beneath the container was previously demonstrated to determine gemcitabine concentration (42.9-58.2 wt%) in the gemcitabine injection powder housed in a glass container. Using the ASI scheme, the spectral features of the gemcitabine powder became distinct with only a weak underlying glass background signal. Meanwhile, since the distance between the laser illumination spot and detector location was increased in the ASI scheme, the attenuation of Raman signal was inevitably large. So, it would not adequate to determine concentration of low-level active pharmaceutical ingredient (API) in a housed pharmaceutical sample due to the degraded signal-to-noise ratio. To secure the enhanced signal-to-noise ratio of API peak, a conventional back-scattering (BC) measurement is preferred; however, the strong presence of glass background is problematic. To increase the intensity of API peak with diminished glass background, BC based ASI (BC-ASI) scheme was explored in this study. The BC-ASI scheme tried to incorporate the advantages of both BC and ASI measurements together in one configuration. Use the BC-ASI scheme, pharmaceutical samples (API concentration below 5.0wt%) housed in a glass vial were measured and subsequent accuracy of API concentration determination was compared with those of BC and ASI measurements.

Oral Presentation : **ANAL1.O-6**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:20

Chair: Yang-Rae Kim (Kwangwoon University)

AutoMRM: a targeted proteomics data interpretation tool based on convolutional neural networks and explainable artificial intelligence

Jungkap Park, Jiwon Hong[1], Seunghoon Back[1], Hokeun Kim[1], Sang-Won Lee[1], Sangtae Kim[2,*]

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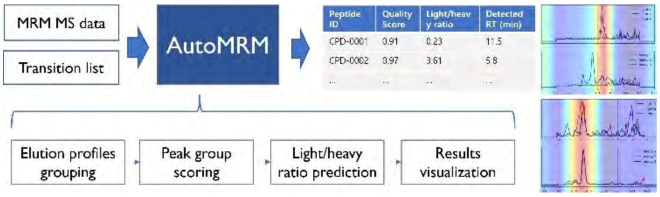
[2]*Bioinformatics Group, Bertis Bioscience Inc., United States*

Deep neural networks have led to breakthroughs in discovery proteomics, but their adoption in targeted proteomics has been slow. In clinical proteomics laboratories, researchers spend a significant time on manual peak picking, interference identification, and peak area adjustments to interpret multiple reaction monitoring (MRM) or parallel reaction monitoring (PRM) data. The burden of manual inspection is a major factor limiting transferability, reproducibility, and scalability of targeted proteomics in clinical applications. We present AutoMRM, a targeted proteomics data interpretation tool based on convolutional neural networks (CNN) and explainable artificial intelligence (XAI), designed for clinical mass spectrometry laboratories. When applied to MRM data, AutoMRM shows an accuracy comparable to that of human experts, obviating or significantly reducing the burden of manual inspection. With AutoMRM, an MRM analysis task which used to take over 600 hours by human experts could be completed in less than 5 minutes. We plan to apply the method to the PRM and data-independent acquisition data.



Peptide ID	Quality Score	Light/heavy ratio	Detected RT (min)
CPD-0001	0.91	0.23	11.5
CPD-0002	0.97	3.61	5.8
...	...	...	...

Oral Presentation : **ANAL1.O-7**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:24

Chair: Yang-Rae Kim (Kwangwoon University)

Investigation of multiple strategies for mass spectrometry based proteomic analysis of bronchoalveolar lavage fluid from lung cancer patients

Minh Hung Vu, Min-Sik Kim[*]

Department of New Biology, DGIST, Korea

Mass spectrometry analysis is a prominent technique for clinical proteomics. Several strategies have been developed to advance biomarker identification from liquid biopsies. Bronchoalveolar lavage fluid (BALF) has recently emerged as a promising source of protein biomarkers for lung cancer. However, challenges due to the properties of BALF have limited the sensitivity and specificity of mass spectrometry-based biomarker identification. Therefore, we systemically investigated different approaches, including sample preparation, peptide fractionation, and data acquisition for quantitative proteomic analysis of BALF from lung cancer patients. Herein, we will address the advantages and caveats of each strategy and propose a potential procedure for biomarker identification from clinical samples.

Oral Presentation : **ANAL1.O-8**
Oral Presentation of Young Analytical Chemists I
Room 201 THU 09:28
Chair: Yang-Rae Kim (Kwangwoon University)

Structural insights into distinct amyloid aggregation dynamics in water and heavy water

MyungKook Son, Dongjoon Im, Dongvin Kwak, Da Gyeong Hyun, Sooyeon Chae, Gyusub Yoon, Chanju Won, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Amyloidosis is a disease related with oligomer-fibrils formed by self-assembly due to misfolding of amyloid proteins. The self-assembly of amyloid protein is achieved through intermolecular hydrophobic interactions, forming the unbranched beta-sheet structured fibrils. The fibrillation process is not easy to study because it has various fibrillation mechanisms that are affected by various biological factors such as pH, metal ions, and temperature. Examples of such amyloid proteins include α-synuclein, tau protein, and amyloid-β associated with degenerative brain disease. These proteins are intrinsically disordered proteins (IDPs) which do not have a distinct structure, and are proteins with a secondary structure, a random coil. Insulin (INS) is related to a injection localized amyloidosis. Contrary to IDPs, INS is a protein with a distinct secondary to quaternary structure. D2O is generally used as a solvent instead of H2O to observe the protein. However, D2O has different physical properties from H2O due to the isotope effect, which may affect the physical properties of proteins. In the first chapter, we investigated the distinct amyloid fibrillation processes of structured protein, human INS, in H2O and D2O using various spectroscopic tools, including 2D-IR spectroscopy. The following chapter discuss the amyloid fibrillation process of intrinsically disordered proteins, α-synuclein and K18. By employing molecular dynamics simulation, an umbrella sampling method, stability of protofibrils in H2O and D2O can be calculated and compared. Overall, this research aims to understand the H-D isotope effect on protein structures and fibrillation kinetics.

Oral Presentation : **ANAL1.O-9**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:32

Chair: Yang-Rae Kim (Kwangwoon University)

Size separation of exosomes and microvesicles by flow field-flow fractionation/multiangle light scattering and the lipidomic comparison

Young Beom Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Extracellular vesicles (EVs) are lipid membrane particles containing proteins, lipids and RNA species. EVs mediate cell to cell communication and are related to immune signaling, cell differentiation and proliferation. Subpopulations of EVs are divided into exosomes (30-100 nm in diameter) and microvesicles (100-1000 nm) and therefore, it is essential to distinguish them separately because they differ in contents, proteins, and lipid compositions. However, isolation of EVs is still not standardized, and each of the EVs separation methods such as ultracentrifugation, size exclusion chromatography, filtration, and precipitation has its own limitations.In this study, separation of exosomes and microvesicles derived from DU145 cells was demonstrated by frit-inlet asymmetrical flow field-flow fractionation (FIAF4) with UV and multi-angle light scattering (MALS) detectors based on field programming. Fractionated exosomes and microvesicles by Flow FFF were confirmed by western blotting and their sizes were determined by MALS calculation and TEM images. Lastly, lipidomic analysis was performed by nanoflow ultrahigh performance liquid chromatography-electrospray ionization-tandem mass spectrometry to investigate the difference in lipid compositions between exosomes and microvesicles which were collected during the FIAF4 runs.

Oral Presentation : **ANAL1.O-10**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:36

Chair: Yang-Rae Kim (Kwangwoon University)

Lipidomic analysis of different aortic macrophages from hyperlipidemic mice by nanoflow ultrahigh performance liquid chromatography tandem mass spectrometry

Jaewon Seo, Gwang Bin Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Lipidomics is a comprehensive study of lipids including identification and quantification of lipids and lipid metabolism. Lipids, being the major components of cell membranes, play essential biological roles such as cell signaling, energy storage, and etc. Because of lipids' diverse roles in biological systems, their abnormal metabolism has been reported to be linked with several metabolic diseases such as diabetes, obesity, and atherosclerosis. Atherosclerosis is a chronic vascular disease characterized by lipid accumulation and subsequent chronic inflammation of the arterial wall. The rupture of advanced atherosclerotic plaques can eventually lead to heart attack and stroke. Since macrophages play essential role at the initial steps of atherosclerosis by turning into lipid-laden foamy macrophages upon ingestion of excessive LDLs, it is important to investigate lipid perturbations between the foamy and non-foamy macrophages from aortas under atherosclerosis. In this study, lipid profiles of three macrophage populations including intimal foamy and non-foamy macrophages and adventitial macrophages of atherosclerotic mouse aortas were analyzed using nanoflow ultrahigh performance liquid chromatography-tandem mass spectrometry. Only 50,000 macrophages of each group were utilized for the analysis and total of 526 lipids were identified and 187 lipids were quantified. As a result, TGs showed different trends in intimal macrophages according to their chain length, while levels of CEs LPCs, and PEs were found to be significantly higher in foamy macrophages compared to non-foamy macrophages.

Oral Presentation : **ANAL1.O-11**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:40

Chair: Yang-Rae Kim (Kwangwoon University)

Optimization of saliva volume for lipid analysis with nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry

Gwang Bin Lee, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Saliva is one of the informative biofluids since it contains enzymes, hormones, and lipids that originated from several sources. The biological molecules in saliva are known to be transferred from blood to saliva. Because of this, saliva is known to have a good correlation with serum and plasma and also reflect the physiological status of the body. In addition, saliva has advantages in sampling; easy-to-collect, non-invasive, and painless compared to serum or plasma. For this reason, human saliva gains much interests to be used to develop effective biomarkers for diagnosing, monitoring disease status, and predicting disease progression. Lipids have highly complex structural diversities and play key tools in biological system such as cell signaling and energy metabolism. Despite its potential as a useful biomarker discovery tool, salivay lipid have been poorly investigated yet. Therefore, it is necessary to optimize the lipid extraction method for saliva.In this study, lipid extracts from various saliva volumes (1.0, 0.5, 0.2, and 0.1 mL) were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). The saliva volumes were evaluated by extraction recovery, matrix effect, and the number of quantifiable lipids. The concentration of each lipid class and lipid species was decreased as the saliva volumes were decreased. The number of quantifiable lipids were 221, 241, 158, and 122 at 1.0, 0.5, 0.2, and 0.1 mL of saliva, respectively. As a result of these, the minimum saliva volume was determined to be 0.5 mL which can perform lipidome analysis effectively by nUHPLC-ESI-MS/MS without losing the number of quantifiable lipids.

Oral Presentation : **ANAL1.O-12**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:44

Chair: Yang-Rae Kim (Kwangwoon University)

Flow field-flow fractionation with thickness tapered channel

SeungYeon Shin, Myeong Hee Moon[1,*]

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Flow field-flow fractionation (FlFFF) is an analytical technique that can separate sample components by sizes with the use of the two flow streams without a stationary phase. Size separation of macromolecules in FlFFF is achieved by the interplay of two perpendicularly moving flows: migration flow (along the channel axis) to transport the sample and crossflow (by the strength of the external field) to retain the sample materials within the channel. Depending on the hydrodynamic diameter, the particles have parabolic flow profiles that are slow near the channel wall and fast at the center. In the steric/hyperlayer mode where particles larger than 1 μm are separated, large particles with higher lift force from the bottom of the channel are located at a faster flow streamline and elute earlier than small particles. Increasing the channel thickness improves the separation efficiency but increased separation time of large particles degrades the sample recovery and resolution. Furthermore, additional flow control equipment and software are required to separate particles in a wide range.In this study, a new type of channel with tapered thickness was introduced to enhance the elution of long retaining sample components in FlFFF. By utilizing a thickness tapered channel, sample migration can be gradually fastened without employing the field programming because the migration flow rate increases along the axis. The separation efficiency of the thickness tapered channel was compared with that of the conventional flat channel by comparing retention time, sample recovery, and steric transition phenomenon under the various flow rate conditions.

Oral Presentation : **ANAL1.O-13**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:48

Chair: Yang-Rae Kim (Kwangwoon University)

Optimization of fecal and saliva sample pretreatment for lipidomic analysis by nanoflow ultrahigh performance-liquid chromatography-electrospray ionization-tandem mass spectrometry

Bo Young Hwang, Jaewon Seo[1], Gwang Bin Lee[2], Myeong Hee Moon[2,*]

department of chemistry, Yonsei University, Korea

[1]*Yonsei University, Korea*

[2]*Department of Chemistry, Yonsei University, Korea*

Lipid profiling for diagnostic purposes has become one of the promising area in relation to metabolomic approach. While most of salivary lipids are originated from serum or plasma, fecal lipids are derived from the gut flora, epithelial cells from the stomach and intestinal tract, and undigested food. Although lipidomic studies about blood and cells have been sufficiently investigated, saliva and fecal lipidomic studies as potential biomarker candidates have not been thoroughly investigated yet.In this study, we have investigated the pretreatment methods of saliva and fecal samples for storage before lipid extraction and the volume of fecal samples needed for lipidomic analysis. Since lipid composition and their levels may change during the transportation between the sampling site and the analytical lab, it is important to investigate the alterations in lipid profile during storage. Saliva samples were exposed in room temperature for 4 days by adding two different types of organic solvents: 95 % EtOH and a mixture of MeOH/MTBE. Lipid profiles of saliva samples treated with organic solvents were evaluated by comparing the normalized peak area of individual lipid species in comparison to that of a fresh saliva sample. Saliva sample mixed with MeOH and MTBE shows the most similar result with the fresh saliva sample than other treatments. Then, Intra Class Correlation (ICC) technique was utilized to verify the degree of maintaining the concentration of lipids in terms of stability and the calculated ICC value was the highest as 0.973 for the saliva treated with MeOH and MTBE condition. In case of fecal samples, the effect of the amount of original feces on lipid identification and quantification was investigated for the optimization, resulting that a. total of 296 lipids were identified from the fecal samples, showing the improvement in lipid identification compared to the reported study.

Oral Presentation : **ANAL1.O-14**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:52

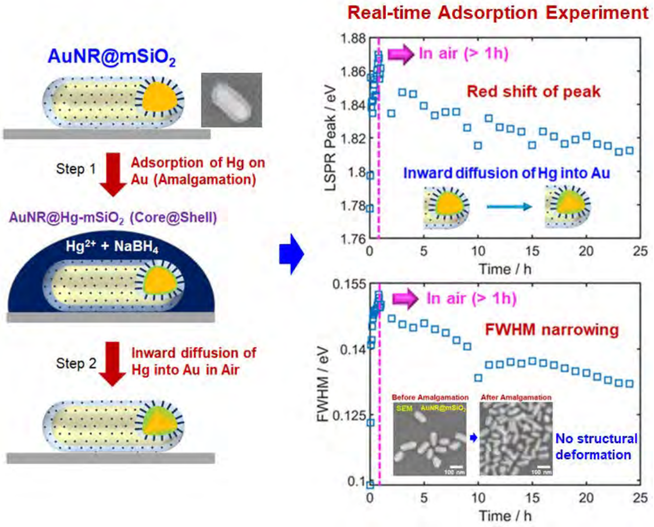
Chair: Yang-Rae Kim (Kwangwoon University)

Single-Particle Study on Hg Amalgamation Mechanism and Slow Inward Diffusion in Mesoporous Silica-Coated Gold Nanorods without Structural Deformation

Geun Wan Kim, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

This paper presents the structural and spectral variations of individual mesoporous silica-coated gold nanorods (AuNRs@mSiO_2) compared to bare AuNRs upon Au-Hg amalgamation. First, the aspect ratio of AuNRs@mSiO_2 exposed to Hg solutions was unchanged because the deformation of the AuNR cores was suppressed by the silica shell. Second, dark-field microscopy and spectroscopy revealed a blue shift of the localized surface plasmon resonance (LSPR) wavelength peak and strong plasmon damping in the scattering spectra of individual AuNRs@mSiO_2 exposed to Hg solutions. Furthermore, we investigated time-dependent adsorption kinetics and spectral changes during Au–Hg amalgam formation in single AuNRs@mSiO_2 over a long timeframe. When AuNRs@mSiO_2 were removed from Hg solution, a gradual red shift and linewidth narrowing of the LSPR peak were observed over time due to the inward diffusion of Hg into the AuNR core. Therefore, this study provides new insights into the relationship among amalgamation process, morphological change, role of silica shell, and LSPR peak and linewidth at the single-particle level.


AuNR@mSiO$_2$
Step 1
Adsorption of Hg on Au (Amalgamation)
AuNR@Hg-mSiO$_2$ (Core@Shell)
Hg^{2+} + NaBH$_4$
Step 2
Inward diffusion of Hg into Au in Air
Real-time Adsorption Experiment
In air (> 1h)
Red shift of peak
Inward diffusion of Hg into Au
LSPR Peak / eV
1.88
1.86
1.84
1.82
1.8
1.78
1.76
0
5
10
15
20
25
Time / h
In air (> 1h)
FWHM narrowing
FWHM / eV
0.155
0.14
0.125
0.1
Before Amalgamation
SEM
AuNR@mSiO$_2$
After Amalgamation
100 nm
100 nm
No structural deformation
0
5
10
15
20
25
Time / h

Oral Presentation : **ANAL1.O-15**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 09:56

Chair: Yang-Rae Kim (Kwangwoon University)

Personal passive air sampler development for measuring chlorinated gases from chlorine-based disinfectants

Yerim Koo, Jung-Hwan Kwon*

Division of Environmental Science & Ecological Engineering, Korea University, Korea

During the COVID-19 pandemic, chlorine-based disinfectants are being widely used at domestic and public places. However, the misuse of chlorine-based disinfectants can generate high concentrations of harmful gases including chlorine gas. Hence, estimating the exposure level of chlorinated gases while using chlorinated disinfectants is necessary. Here, we developed a personal passive air sampler (PPAS) composed of *o*-dianisidine and a polydimethylsiloxane (PDMS) sheet: *o*-dianisidine which is doped inside the PDMS changes its color due to the oxidation reaction with chlorinated gases. Thus, the PPAS developed in this study allow to detect personal exposure to the chlorinated gases by the naked eyes, while cumulative exposure could be determined by measuring reduced mass of *o*-dianisidine after exposing to the chlorinated gases. By a chamber test, calibration of PPAS was successfully conducted with obtaining a sampling rate of 0.00253 m^3/h. Color development of the passive sampler corresponding to chlorine exposure concentration and time was also investigated. Finally, a panel study was conducted with the help of ten volunteers who were asked to clean their bathrooms with household chlorinated disinfectants. Each panel wore the PPAS during their cleaning work, and the personal exposure level was effectively estimated after the extraction of *o*-dianisidine in the PPAS. Thus, we confirmed that the PPAS can be useful for detecting personal exposure to chlorine-based gases during indoor sanitation including COVID-19 disinfection.

Oral Presentation : **ANAL1.O-16**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:00

Chair: Yang-Rae Kim (Kwangwoon University)

Optically Pumped and Matrix Assisted Anti-Stokes Raman Spectroscopy

Si Won Song, Jin Il Jang, Chan Ryang Park, Hyung Min Kim[*]

Department of Chemistry, Kookmin University, Korea

Anti-Stokes Raman spectroscopy is an excellent method to suppress optical backgrounds from Raman scatters and sur-rounding materials, even in electronic resonance conditions. The upshift of scattered light can avoid the fluorescence or phosphorescence that is usually red-shifted with respect to the excitation wavelength. However, this method's competence is circumscribed by its low scattering efficiency, which results from an insufficient population of upper vibrational states that obey temperature-dependent Boltzmann statistics. To overcome this limitation, we propose that the mode-selective absorption of overtone or combination vibrations leads to enhanced anti-Stokes Raman scattering under simultaneous near-infrared (NIR) pumping and Raman excitation. Particularly, vibrationally resonant pumping is efficient for population transfer, and the excess energy is thermodynamically distributed over all fundamental vibrations. Furthermore, we present that NIR absorbing molecules can be employed as matrices to amplify anti-Stokes Raman signals of weak scattering targets.

Oral Presentation : **ANAL1.O-17**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:04

Chair: Yang-Rae Kim (Kwangwoon University)

Time series evaluation of the diagnostic index Optical Redox Ratio

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Autofluorescence is a non-invasive analysis method which is used to diagnosing for in vivo and ex vivo tissues. Optical Redox Ratio (ORR) is a value obtained through the ratio of fluorescence intensity of Nicotinamide dinucleotide (NADH) and Flavin adenine dinucleotide (FAD). NADH and FAD are co-enzymes used in metabolism and respirations, which are strongly associated with pathological symptoms, so ORR is used as indicators for diagnosing lesion and cancer tissue. However, ORR has a various result of research on tissues and few reports have been reported on evaluating the variation of ORR value over time. In this study, we measured absorption and fluorescence over time by preparing a mixed solution of NADH and FAD at concentrations similar to biological conditions for evaluation of ORR indicators. The ORR value was obtained by decomposing each spectrum of NADH and FAD in the spectrum of the mixed solution. It was observed that the fluorescence spectral region of NADH decreased and FAD was uniform over time. This is due to the oxidation-reduction coupled reaction of NADH and FAD. In addition, fluorescence intensity of both NADH and FAD decreased when measuring fluorescence, which is an effect by the inner filter effect, and these effects tend to increase ORR values over time. Based on the spectroscopic study, we concluded that ORR values need to be calibrated before using them as a spectroscopic diagnostic marker.

Oral Presentation : **ANAL1.O-18**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:08

Chair: Yang-Rae Kim (Kwangwoon University)

Analysis of Korean ancient glasses using Raman Spectroscopy

Wooseok Sim, Hyung Min Kim[1,*], Gyuho Kim[2,*]

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[2]*Cultural Heritage Conservation Science, Kongju National University, Korea*

Korean ancient glasses are significantly important historical sources. Especially, to know components of ancient glasses can help us determine the distribution network, the technical skills of our ancestor and the period when ancient glasses were produced. Generally, the instruments that are used to determine components of ancient glasses are ED-XRF(Energy dispersive X-Ray Fluorescence Spectrometer), EDS(Energy dispersive X-ray spectrometer) and so on. Those instruments are great tools to analyze components of ancient glasses. Operating ED-XRF, however, the samples must be under vacuum and using EDS, the samples must be preprocessed, which can be not only bothersome and time-consuming but cause destruction of samples. Although finding out the components of ancient glasses is significant, cultural assets should be conserved. Therefore, nondestructive analysis techniques are key factor to do research on cultural properties. In terms of nondestructive analysis, Raman Spectroscopy is a powerful tool. For these reasons, we employed Raman Spectroscopy to determine components of Korean ancient glasses and classify those. A 532 nm laser was used to analyze Korean ancient glasses. Depending on the groups of each glass, we could get different Raman spectra, which is caused by the differences of cation that was melted into glasses. We compared Raman spectra with EDS data and we could confirm that Raman spectroscopy can give us accurate information on qualitative analysis of ancient glasses. In addition, we suggested the possibility that by using Raman Spectroscopy we can determine the quantification information about PbO components in the lead glasses. Consequently, we note that based on Raman spectra we can do qualitative and quantitative analysis of the Korean ancient glasses.

Oral Presentation : **ANAL1.O-19**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:12

Chair: Yang-Rae Kim (Kwangwoon University)

Quantification for unopened milk via multi-offset SORS probe

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Health has been a hot issue for worldwide people for last century and industries for health care has been grown dramatically. In particular, the interest in obesity has made people interested in fat content in food, even some countries, such as the United States and EU, recommend a low-fat diet. Accordingly, measuring the fat content of food is an important issue, and the development of its non-destructive and fast analysis method is inevitable. For the above reasons, we decided to analyze the fat content in food. Among many foods, the sample we chose is milk that is familiar and can be found in our everyday life. It also has an advantage in cost.Generally, using chromatography like GC or LC provides good enough quantitative information, but chromatography analysis is expensive, need much time, and limited in analysis without opening the milk pack. On the other hand, Raman spectroscopy is not only fast, portable, but also has the potential to analyze components in packaged materials without opening the packaging. That`s why we select SORS(Spatially Offset Raman Spectroscopy), a kind of Raman spectroscopy, the most suitable method for analyze unpacked milk. The SORS which can overcome Raman interference in the package to detect internal substances is a method for profiling depth information. In this study, we developed a line mapping multi-offset Raman probe system for quantitative analysis of fat that analyzes milk fat without opening the package. The line mapping multi-offset Raman probe system will provide accurate milk quantification information. In addition, our systems enable on-site analysis for suppliers, markets and consumers in dairy industry.

Oral Presentation : **ANAL1.O-20**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:16

Chair: Yang-Rae Kim (Kwangwoon University)

Optimization of urinary small extracellular vesicle isolation using multiple cycles of centrifugation

Iqbal Jalaludin, Jeongkwon Kim*

Department of Chemistry, Chungnam National University, Korea

Small extracellular vesicles (sEV), particularly exosomes, are cell-released nanoparticles that deliver bioactive components to recipient cells, influencing the cell’s biological properties. Many studies have shown that sEV has a role in regulating physiological and pathological processes, indicating its functions as a mediator for intercellular communication. Several approaches for sEV isolation have been developed. One of the approaches is multiple cycles of centrifugation (MCC), which is similar to ultracentrifugation (the gold standard for sEV isolation) but uses a lower centrifugal speed and more centrifugation cycles. We optimized the MCC method to isolate sEV from urine by characterizing the size and related components that confirmed the presence of sEV using BCA protein assay, 1D gel electrophoresis, Western blotting, dynamic light scattering and mass spectrometry (MS). Our findings revealed that four cycles of centrifugation were sufficient to separate urine sEV, as shown by the BCA assay and ID gel analysis, where the concentration of proteins of the centrifugation cycle before the final isolated pellet was significantly reduced. The presence of sEV was confirmed by Western blotting that displayed a strong band of CD63 and TSG101 antibodies. The particle size of the final cycle was consistent between 50 and 200 nm, reflecting the typical size of sEV. A comparison of the MS spectra of supernatants and pellets showed differences in spectra profiles. After each centrifugation, MS peaks were reduced in supernatants, while the final pellet contained unique peaks associated with sEV. In this study, the MCC strategy was employed to establish the basis for future urine sEV research, particularly in the facility that lacked advanced instrumentation.

Oral Presentation : **ANAL1.O-21**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:20

Chair: Yang-Rae Kim (Kwangwoon University)

Raman spectroscopic identification of different rice brands

Thu thuy Bui, Seongsoo Jeong, Haeseong Jeong, Hoeil Chung*

Department of Chemistry, Hanyang University, Korea

ST25 rice is a premium Vietnamese rice. The grain of ST25 rice is long with fragrance and has an appealing pineapple flavor. Moreover, since the protein content in ST25 rice is high, it becomes more attractive to people with diabetes as well as those concerning nutrition balance. Due to the high price of ST25 rice, blending with other rice varieties to gain more profits in the current market is inevitable. Therefore, to secure customer trust in purchase of goods, its authentication in market becomes more demanding and non-destructive analytical tools meeting the demand are desirable. Therefore, Raman spectroscopy able to provide rich compositional information of rice samples has been suggested. Initially, Raman spectra of ST25 and non-ST25 rice samples were acquired with sample rotation for representative spectroscopic sampling and their spectral features were comparatively analyzed. Then, the discriminability of ST25 rice samples in a principal component (PC) score domain was assessed. Meanwhile, when temperature of rice sample change, temperature-induced molecular vibrations of rice constituents is dissimilar and accordingly varied spectral feature of the sample would be more sample-to-sample characteristic. With this motivation, Raman spectra of the samples collected at different temperatures were used for analysis and subsequent discrimination results compared. Finally, two-dimensional (2D) correlation analysis effectively recognizing the temperature-induced spectral variation was adopted to potentially improve the discrimination further.**Keywords:** ST25 rice; Raman spectroscopy; Non-destructive analysis; Temperature perturbation; Two-dimensional correlation analysis

Oral Presentation : **ANAL1.O-22**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:24

Chair: Yang-Rae Kim (Kwangwoon University)

Development of High Resolution 29Si MRI imaging probe based on 29Si Isotope-Enriched Silicon and Silica nanoparticles

Jiwon Kim, InCheol Heo[1], TaeHo Jang[2], Won Cheol Yoo[3,*], Youngbok Lee[4,*]

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Dynamic nuclear polarization (DNP) technique is considered as a potential method for amplifying sensitivity of magnetic resonance (MR) imaging. Recently silicon and silica nanoparticles are in the spotlight as DNP-MRI image probes due to their biocompatibility, but 29Si MR imaging is still limited due to the insufficient hyperpolarization of nano-sized silicon nanoparticles (SiNP) and the lack of electronic defects in silica nanoparticles (SiO2 NP). To overcome the current challenges, we fabricated 29Si-enriched (10%, 15%) porous Si NPs (160 nm) and selectively 29Si-enriched core-shell SiO2 NPs by using 100% 29Si-TEOS. The physicochemical properties of particles were confirmed by SEM, TEM, and XRD. In particular, SiO2 NPs were prepared by designing a core of 40 nm and a shell of 10 nm to demonstrate the microwave penetration depth, and it was confirmed that the core-shell structure was well formed through SEM analysis. As results of DNP experiment in Si NPs, 15% enriched NPs represented ~16 times signal enhancement over natural abundance sample due to the high 29Si ratio. Furthermore, phantom imaging and animal administration were performed to demonstrate the usability of 15% 29Si-enriched particles as MRI imaging probe.In the case of core-shell SiO2 NPs, it was affirmed that the higher 29Si enrichment ratio, the improved signal enhancement, and the penetration depth of the microwave radiation was proved to about 10 nm. Currently, we are conducting research on designing particles with high signal intensity and appropriate T1 time by using TEMPOL-TEOS to select particles that can be used for MRI application.This further study is expected to increase the usability of in vivo MR imaging of SiO2 NPs by enabling self-polarization.

Oral Presentation : **ANAL1.O-23**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:28

Chair: Yang-Rae Kim (Kwangwoon University)

Sensitive detection of SARS-CoV-2 antigen using SERS-based lateral flow assay kit with portable Raman reader

Younju Joung, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

SARS-CoV-2 has spread worldwide for over two years now. Reverse transcription-polymerase chain reaction (RT-PCR) has been considered a gold standard method for detecting the SARS-CoV-2 target gene. In RT-PCR, however, the total diagnostic time takes approximately 3-4 hours. Thus, it is necessary to shorten the detection time for rapid on-site diagnosis. Rapid antigen test kits using antigen-antibody reactions were also developed to shorten the detection time. However, they have not been adopted as a standard method due to their low sensitivity and poor accuracy. In particular, the false-negative problem of commercial rapid antigen test kits is recognized as a severe problem that can aggravate the spread of the SARS-CoV-2. To resolve this issue, we have developed a surface-enhanced Raman scattering (SERS)-based lateral flow assay (LFA) kit with a portable Raman reader for rapid and sensitive detection of SARS-CoV-2 antigen. The SERS-LFA was performed SARS-CoV-2 lysate in a viral transport medium containing nasopharyngeal swab with different concentrations of the virus (0 – 1,000 PFU/mL) and had a limit of detection (LoD) of 3.53 PFU/mL. The SERS-LFA test of SARS-CoV-2 patients was also performed for 33 clinical samples (28 positives and 5 negatives). Our SERS-based lateral flow assay kit shows a strong potential to resolve the problems in terms of low sensitivity inherent in conventional rapid kits to detect SARS-CoV-2.

Oral Presentation : **ANAL1.O-24**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:32

Chair: Yang-Rae Kim (Kwangwoon University)

Surface-enhanced Raman scattering-based lateral flow assay strip for simultaneous diagnosis of SARS-CoV-2 and influenza A infections

Mengdan Lu, Younju Joung, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

There is a high possibility that the seasonal flu is likely to spread simultaneously with severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) owing to the extended duration of the worldwide spread of COVID-19. Because SARS-CoV-2 and influenza A present similar symptoms, they are not easily distinguished without an accurate diagnosis. Therefore, when a person exhibits signs of infection, it is critical to rapidly and accurately determine which virus has infected them and initiate appropriate treatments. A colorimetric lateral flow assay (LFA) strip that can diagnose these conditions simultaneously is commercially available; however, its poor sensitivity causes a false-negative diagnosis problem. To address this, a surface-enhanced Raman scattering (SERS)-LFA strip that can simultaneously diagnose SARS-CoV-2 and influenza A with high accuracy has been developed in this study. This SERS-LFA strip provides a 100- to 1000-fold higher diagnostic sensitivity than the conventional colorimetric LFA strip. Meanwhile, it also has good clinical performance. Therefore, it is possible to identify SARS-CoV-2 and influenza A rapidly and accurately using SERS-LFA strips. Furthermore, this strip is expected to dramatically improve the false-negative diagnoses of early-stage or asymptomatic infections.

Oral Presentation : **ANAL1.O-25**

Oral Presentation of Young Analytical Chemists I

Room 201 THU 10:36

Chair: Yang-Rae Kim (Kwangwoon University)

SERS-based ELISA assay for Sensitive SARS-CoV-2 Detection Using Silica-encapsulated Au Core-Satellite Nanoparticles

Qian Yu, Hoa Duc Trinh, Sangwoon Yoon[*], Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

The enzyme-linked immunosorbent assay (ELISA) is the most widely used immunoassay technique to detect an antigen or its complementary antibody. However, sometimes it does not show sufficient sensitivity. A high-sensitivity immunoassay technique based on surface-enhanced Raman scattering (SERS)-ELISA using plasmonic nanoparticles was developed to overcome the limit of sensitivity inherent in conventional ELISA. In SERS-ELISA, SERS nanotags adsorbed to the surface of metal nanoparticles with Raman reporters were used as detection labels. When SERS nanotags are exposed to a laser beam, the incident beam intensity is dramatically enhanced by the electromagnetic enhancement effect in hot spots. Using this phenomenon, the problem of low sensitivity, inherent in conventional absorption or fluorescence ELISA, could be solved. In SERS-ELISA, however, it is critical to develop functional nanoparticles that control hot spots to realize high sensitivity and reproducibility. In this work, a silica-encapsulated core-satellite Au naoparticles (CS@SiO$_2$) has been developed for the sensitive detection of SARS-CoV-2. In addition, the assay was performed using a 384-well plate instead of a 96-well plate to reduce the sample amount. As a result, the low limit of detection (LOD), 8.81 PFU/mL, could be obtained, which exhibited eight times better sensitivity than a traditional ELISA. We believe that this SERS-ELISA technique has a strong potential to be a powerful tool for diagnosing various infectious diseases in the future.

Oral Presentation : **ANAL2.O-1**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:00

Chair: Jongcheol Seo (POSTECH)

Mesoporous Silica-Polydopamine Janus Nanoparticles for Removal Spontaneous Organic Pollutants in Oil/Water Phase

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[1]*Department of Bio-Nano Technology, Department of Applied Chemistry, Korea*

Due to dual compositions and capabilities, mesoporous Janus nanoparticles (mJNPs) have been exploited in a variety of applications including biomedicine, catalysis, and energy storage; nevertheless, their low surface area remains a barrier. As a result, we present spherical or bowl mesoporous polydopamine (mPDA) and spherical mesoporous silica (mSiO2) Janus nanoparticles with high surface area and surface modification, which were synthesized using the Volmer-Weber heterogeneous nucleation approach. The mPDA was produced as a spherical or bowl shape using an emulsion anisotropic assembly process with a size range of 200 nm to 300 nm. The spherical mSiO2 has a diameter of 100 nm, as determined by scanning electron microscopy (SEM). The Infrared spectroscopy (FT-IR) and nitrogen adsorption-desorption (BET) were used to confirm their chemical and physical characteristics. Finally, these Janus nanoparticles were used in wastewater treatment experiments with single and dual contaminants. In order to remove spontaneous organic pollutants in the oil-water phase, we used a Pickering emulsion system of mJNPs.

Oral Presentation : **ANAL2.O-2**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:04

Chair: Jongcheol Seo (POSTECH)

Investigation of DNP Spin Diffusion Barrier for TEMPOL Radical Embedded Silica Nanoparticles

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Dynamic Nuclear Polarization is a hyperpolarization technique which can be used to greatly amplify NMR signals. The hyperpolarization requires free electrons in order to create electron spins polarization which is then transferred to nuclear and enhance the nuclear spins polarization. In terms of silica nanoparticles, due to the absence of unpaired electrons, the use of exogenous species, like TEMPOL, is necessary to provide the particles with free electrons. Normally, TEMPOL is added externally into the silica powder before DNP measurement, but this leads to the limited polarization extent from particles surface (~4.2 or ~5.7 nm). In this study, we synthesized the small size TEMPOL embedded silica nanoparticles (~80nm) with homogeneous and core-shell structures for DNP measurement to investigate the nuclear spins polarization enhancement, especially, the homogeneous particles with the regular distribution of TEMPOL radicals inside can induce the polarization of the whole particles. The EPR results of synthesized silica nanoparticles confirmed the presence of TEMPOL radicals attached in the particles. In addition, the NMR measurements showed that the TEMPOL adding almost has no significant impact on the silica peaks. These results showed the promising of using these particles for further DNP experiments.

Oral Presentation : **ANAL2.O-3**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:08

Chair: Jongcheol Seo (POSTECH)

Investigation of pH-Responsive Microcapsule based on Natural Polymers with High Applicability in Cosmetic Products

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Nowadays, functional hydrogels based on hyaluronic acid are gaining much attention because of their high applicability in cosmetics, pharmaceuticals, or foods. However, not many studies could control the shape and size of microcapsules based on this material using simple methods such as coacervation method, so we attempt to fabricate small-sized functional microcapsules with perfectly spherical shapes and investigate their intriguing stimulus-response properties. Our core-shell microcapsule is synthesized by complex coacervation method using natural polymers including sodium alginate (SA), hyaluronic acid (HA), and gelatin (GEL) as wall materials which protect active agent, vitamin E, present in core. Morphology and particle size of synthesized microcapsule were characterized by microscopy, interactions inside of microcapsule's structure were predicted through IR measurement, and UV spectroscopy also is used in encapsulated-vitamin E determination. According to microscope images, microcapsules are spherical and uniform, particle size around 20 µm to 30 µm, which is tunable by changing the HA component. Moreover, HA showed high potential in enhancing encapsulation efficiency of microcapsule, which was elucidated when EE% reached 73.8% with 1.0% w/v of HA appearance, but it only achieved 35.7% in the case of the conventional system. In addition, swelling behavior experiment performed based on the change in particle size showed microcapsules having a high swelling degree at pH 5.5, demonstrating pH-responsive characteristics of microcapsules. For further research, we will investigate more experiments to verify this microcapsule's biocompatibility and biodegradability, such as in vitro and in vivo examinations.

Oral Presentation : **ANAL2.O-4**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:12

Chair: Jongcheol Seo (POSTECH)

Determination of Double-bond Position in Unsaturated Lipids by Ozonolysis Paper Spray Ionization Mass Spectrometry (OzPSI MS)

Youngjoo Kal, Sangwon Cha*

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Lipids are essential biomolecules as major components of cell membranes and energy sources. For lipid characterization, mass spectrometric methods have become a major workhorse, but it is hard for mass spectrometry (MS) to distinguish isomers or locate double bond(s) without employing a tandem MS (MS/MS) approach. In this study, we developed an ambient ionization platform to determine double-bond position in unsaturated lipids without performing a tandem MS experiment. The platform mainly consists of paper spray ionization (PSI), one of the simplest ambient desorption ionization methods with liquid extraction based desorption process, and an ozone-producing UV lamp. So, we called this platform ozonolysis PSI MS (OzPSI MS). Ozone produced by low pressure mercury lamp induced the cleavage at carbon double bond in lipids to form aldehyde terminals or carbonyl oxide terminals. Double bond position could be located by observing these ozonolysis products without performing tandem MS. Examples with phospholipids and long-chain fatty acids will be demonstrated in this presentation.

Oral Presentation : **ANAL2.O-5**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:16

Chair: Jongcheol Seo (POSTECH)

Rapid Analysis of Proteins by Droplet Paper Spray Ionization Mass Spectrometry (Drop-PSI MS) with a Hydrophobic Paper Tip

Sungjun An, **Sangwon Cha**[*]

Department of Chemistry, Dongguk University, Korea

This study investigates the use of paper spray ionization (PSI), a fast and simple ambient desorption ionization technique for mass spectrometry (MS) for rapid detection and analysis of proteins. Since a conventional cellulose-based paper substrate is too hydrophilic for proteins to be desorbed and ionized in a PSI process, various modifications on a paper substrate to increase its hydrophobicity have been suggested. Instead of modifying a paper tip in house, we tested various synthetic and natural paper that are commercially available for protein detection by PSI MS. We found that a Teslin paper, a synthetic microporous polyolefin silica matrix substrate, served as an excellent PSI tip for proteins. Since highly aqueous sample solution stays as a droplet on a Teslin PSI tip, we called this technique droplet PSI MS (Drop-PSI MS). In Drop-PSI MS, rapid protein analysis could be achieved in a 'drop and go' fashion and in situ modification of a sample solution was feasible. Examples of protein analysis on various PSI platforms will be demonstrated and compared. In addition, advantages and limitations of Drop-PSI MS will be highlighted and discussed in this presentation.

Oral Presentation : **ANAL2.O-6**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:20

Chair: Jongcheol Seo (POSTECH)

In Situ Separation and Analysis of Bile Juice Using Paper Spray Ionization Mass Spectrometry

Donghoon Lee, Eunjin Jang[1], Hoeil Chung[1], Sangwon Cha[*]

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Paper spray ionization (PSI), a simple ambient ionization method for the mass spectrometry (MS), has been employed for the rapid chemical fingerprinting analysis of the biofluid samples such as urine, blood and serum. In this study, PSI MS was employed for the analysis of the various metabolic components present in a bile juice sample, such as bile salts, phospholipids, proteins, fatty acids, and bilirubin-derived chemicals. For PSI MS analysis, one microliter of diluted bile juice was spotted onto a triangular paper tip and dried without further sample pretreatment. We tested various types of spray solvents against a bile juice sample in order to find the optimized PSI condition in terms of sensitivity and metabolite coverage. In addition to simple fingerprinting experiments, we tried to separate bile juice metabolites according to their classes during analyte transportation process in PSI. Bile salts, the most polar components in bile juice, could be clearly separated and detected from phospholipids by feeding a spray solvent into a paper tip. Our study demonstrated that PSI-MS could serve as the fast chemical fingerprinting platform for bile juice metabolites and was also able to provide wide metabolite coverage through the in-situ separation capability.

Oral Presentation : **ANAL2.O-7**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:24

Chair: Jongcheol Seo (POSTECH)

Towards the Laboratory Automation: From the 3D Printer Modifications

Hwa-yong Jang, Han Bin Oh*

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In this study, an open-source fully automated sample preparation robot manufactured from a modification of a 3D printer was developed to be used for liquid chromatography/mass spectrometry (LC/MS) analysis. This robot was designed to perform a series of well-organized sample pretreatment steps such as micropipetting, gripping, vortexing, centrifugation, and heating block shaking without human intervention. In addition, since the auto-storage modules and transfer modules that can automatically supply the reagents required for the pretreatment process and storage the samples after the experiment have been completed, were also developed, it is able to automate whole sample preparation steps. Further, all the information needed for the fabrication, including design files, are open to the public.

Oral Presentation : **ANAL2.O-8**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:28

Chair: Jongcheol Seo (POSTECH)

Optimization of Headspace Gas Chromatography-Mass Spectrometry (HS-GC-MS) for Nontarget Analysis of Various Forms of Household Chemical Products

Yougyeong Park, Sangwon Cha*

Department of Chemistry, Dongguk University, Korea

We are exposed to numerous household chemical products (HCPs) in our daily lives. Our health status could be significantly affected by this exposure since HCPs possess various highly volatile chemicals releasing to our living environment. Therefore, analysis of volatile chemicals, not limited to known components, from HCPs are essential for health risk assessment of HCPs. In this study, we developed a nontarget analysis (NTA) platform for volatile chemicals in HCPs with headspace gas chromatography-mass spectrometry (HS-GC-MS). Three different types of HCPs, liquid and powder detergents, and fabric softener sheet, were employed for optimization of sample preparation and HS conditions. In other words, different sample pretreatments and HS procedures like equilibration time and temperature were tested for each formula. In order to investigate the performance of the HS procedure, we compared our HS-GC-MS method with an offline solid phase extraction (SPE) followed by GC-MS. We found that our HS approach induced much less contamination during sample preparation and analysis, provided the better coverage for volatile compounds, and showed the greater reproducibility and confidence in identification than the approach with an offline extraction and GC-MS.

Oral Presentation : **ANAL2.O-9**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:32

Chair: Jongcheol Seo (POSTECH)

Characterizing the Optical Properties of Hollow Gold Nanoshells with Plasmonic Effect

Yun a Hong, Ji Won Ha*

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Plasmonic gold nanoparticles are widely used as the sensor because of localized surface plasmon resonance (LSPR) effect. LSPR is the collective vibration of the surface conducting electrons when light is incident to the gold nanoparticles, along with the incident electromagnetic field. Among many gold nanoparticles, hollow gold nanoshells (HGNs) are hollow and consists of a thin gold shell and has a wider linewidth than other types of gold nanoparticles. Furthermore, HGNs have received great interest in the fabrication of biosensors due to several advantages over the solid counterparts such as high specific surface, low density, and reduction of costs. In this study, we employed dark-field (DF) spectroscopy that is a powerful tool that can visualize individual gold nanoparticles and determine their homogeneous LSPR spectra. We investigated scattering properties of single HGNs and the amplification of Raman scattering intensity by molecules chemically adsorbed on the metal surface. Therefore, we provide a deeper understanding of the characteristic optical properties of single HGNs under DF and Raman spectroscopy.

Oral Presentation : **ANAL2.O-10**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:36

Chair: Jongcheol Seo (POSTECH)

The Effects of Chemisorption on Refractive Index Sensitivity in Mesoporous Silica Coated Gold Nanorod

Seongeun Heo, Ji Won Ha[1,*]

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Gold nanoparticles have unique optical properties depending on their shape, size, and the refractive index of surrounding medium, caused by local surface plasmon resonance (LSPR) effect. Because of these characteristics, it is currently used in various fields such as drug delivery, photothermal therapy, biosensor, etc. In this study, we characterized mesoporous silica coated gold nanorods (AuNRs@mSiO_2), one of the gold nanoparticles with silica shell. We used dark-field (DF) microscopy and surface enhanced Raman scattering (SERS) to investigate the optical properties of single AuNRs@mSiO_2. We studied the LSPR sensitivities of two different sizes of single AuNR@mSiO_2 toward changes in the three different refractive indices (RI) of surrounding medium (air, water, oil). In addition, we used the derivative methods to improve RI sensitivity by using the inflection point. Therefore, this study provides a deeper understanding of characteristic scattering properties of AuNR@SiO_2 with different sizes as well as the effect on their RI sensitivity at the single particle level.

Oral Presentation : **ANAL2.O-11**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:40

Chair: Jongcheol Seo (POSTECH)

The efficacy of prostate cancer diagnosis using PSA between blood test and cancer tissues

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As a protein biomarker, prostate-specific antigen (PSA) in blood has been widely used for the early diagnosis of prostate cancer (PCa) in clinics. However, PSA also increases in other prostate diseases, such as benign prostatic hyperplasia (BPH) and prostatitis. This leads to a higher number of false positives and causes unnecessary biopsies, an invasive procedure which is associated with risks including bleeding and sepsis. This study intended to identify PSA information from different prostate cancer tissues with different PSA values in patients' blood to discover relationship between blood and cancer tissues for a more accurate early diagnosis.PCa tissues were collected from the PCa patients, homogenized, and proteins were extracted from the homogenized PCa tissues. Then each supernatant fluid was trypsin digested and desalted respectively, and the proteins in all PCa tissues were identified and quantified using nLC-MS/MS and protein database search softwares.

Oral Presentation : **ANAL2.O-12**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:44

Chair: Jongcheol Seo (POSTECH)

Single-Particle Spectroelectrochemistry: Electrochemical Tuning of Plasmonic Properties via Mercury Amalgamation in Mesoporous Silica Coated Gold Nanorods without Structural Deformation

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This paper presents the elucidation of the mercury (Hg) amalgamation induced by electrochemical reduction on gold nanorods coated with mesoporous silica shell (AuNRs@mSiO_2) by single-particle spectroelectrochemistry. First, the silica shell significantly enhanced the structural stability of AuNR cores after Hg amalgamation with application of linear sweep voltages (LSVs). Thus, it became possible to focus on the spectral changes of AuNRs@mSiO_2 induced by the deposition of Hg without disturbance of structural deformation that also strongly affects the localized surface plasmon resonance (LSPR) properties. Second, following the application of LSV in the presence of Hg^{2+}, a remarkable blue shift of LSPR peak was observed, caused by lowering of the work function due to the Hg adsorption, donating electron density to Au. Furthermore, the LSPR linewidth also showed a dramatic increase after the Hg deposition with LSV. Last, direct observation of the evolution of the Hg amalgamation process was presented by monitoring real-time LSPR peak and LSPR linewidth shifts of single AuNRs@mSiO_2 in the Hg solution according to application of electrochemical potential. Moreover, the results showed the possibility of in-situ tuning of the LSPR properties of AuNRs@mSiO_2 by the Hg deposition via electrochemical potential manipulations without disturbance of structural variations of AuNR cores.Keywords: Spectroelectrochemistry, Au-Hg amalgamation, Gold nanorods, Mesoporous silica shell, Single particle spectroscopy, Localized surface plasmon resonance

Oral Presentation : **ANAL2.O-13**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:48

Chair: Jongcheol Seo (POSTECH)

Metabolomic analysis in liver tissues from mouse model to determine the role of AMPK activator in NASH using LC-MS

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Non-alcoholic steatohepatitis (NASH) is a risk factor for hepatocellular carcinoma lead to liver cell damage and inflammation along with fatty deposition. AMP-activated protein kinase (AMPK) plays an important function in controlling energy homeostasis and the activation can inhibit NASH pathology. However, the effect of the AMPK activation on hepatic metabolic rewiring remains unknown.This study aimed to investigate the therapeutic effects of AMPK on hepatic metabolism on NASH using metabolic analysis. C57BL/6J male mice were fed a choline-deficient high fat diet (CD-HFD) for 6 weeks to induce NASH and treated them with YE-21, a new direct AMPK activator candidate, every 2 days for 14 times. Then, we performed metabolic profiling of liver tissue using ultra-performance liquid chromatography–quadrupole time-of-flight mass spectrometry. Mice were divided into four groups: control (n=12), YE-21 (n=12), CD-HFD (n=12), and CD-HFD+YE-21 (n=12). We observed strong separation among three groups of control, CD-HFD and CD-HFD+YE-21 mice in partial least squares-discriminant analysis score plots. A total of 92 metabolites were identified in positive and negative mode. To find key metabolic pathways after YE-21 treatment in mice fed CD-HFD, pathway analysis was performed using significantly different 17 metabolites between CD-HFD and CD-HFD+YE-21. As a result, the most enriched metabolic pathways were cysteine and methionine metabolism, pyrimidine metabolism and amino sugar and nucleotide sugar metabolism. In particular, s-adenosyl homocysteine significantly increased in CD-HFD+YE-21 compared to CD-HFD, whereas cystathione and glutathione oxidized (GSSG) were significantly decreased in CD-HFD+YE-21 compared to CD-HFD in cysteine and methionine metabolism. Our finding suggested that YE-21 might improve liver damage and fibrosis due to NASH by regulating hepatic metabolism, and demonstrated that metabolic profiling is a useful method to investigate the therapeutic effects of AMPK activation in diet-induced NASH mice.

Oral Presentation : **ANAL2.O-14**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:52

Chair: Jongcheol Seo (POSTECH)

Crosslink of metabolic alternations between liver and adipose tissues in mouse models with nonalcoholic steatohepatitis (NASH)

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Nonalcoholic fatty liver disease (NAFLD) is recently recognized as one of the most prevalent etiologies of chronic liver disease, affecting 25% adult population worldwide. NAFLD represents a wide spectrum of diseases ranging from nonalcoholic fatty liver (NAFL) and the progressive form as nonalcoholic steatohepatitis (NASH). However, there is a lack of investigation summarizing organ metabolic changes in NASH model. In this study, we examined the metabolic changes in liver and adipose tissues of mice (n=47) using liquid chromatography/triple quadrupole mass spectrometry (LC/TQ-MS) for polar extracts. Control group was fed with chow diet for 3 weeks whereas NASH groups were fed with high fat diet (HFD) for 3,10,33 and 43 weeks, and mice were sacrificed at each time point. Total 8 classes of polar metabolites were found from semi-targeted polar analysis and then Mann-Whitney test was performed to compare alternations between group and ahead group along NASH progression in liver and adipose tissues. For polar metabolites, amino acids represented similar trend along the period of NASH diet fed in liver and adipose tissues. Intriguingly, change of branched chain amino acids and aromatic amino acids first appeared in liver tissues compared with in adipose tissues. This study demonstrates LC-MS/MS based metabolic profiling is a useful tool to detect characteristic changes along HFD feeding period in liver and adipose tissues.

Oral Presentation : **ANAL2.O-15**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 09:56

Chair: Jongcheol Seo (POSTECH)

Metabolomic analysis of brain tissues from mice exposed to ambient particulate matter using LC-MS approach

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Ambient particulate matter(PM) has become major environmental risk factors to public health, and related to human diseases including respiratory disease, cardiovascular and nervous disorder. However, the effect of exposure to PM has not been fully understood in a biological system. We observe the metabolic changes in response to PM with a diameter 2.5-10 μm (PM10) exposure in mouse model.In this study, C57BI/6J mice (male) were exposed to PM10 or clean air for 3 weeks in chambers. We conducted a targeted analysis of cortex and cerebellum from mice to assess the metabolic perturbations using ultra performance liquid chromatography/triple-quadrupole mass spectrometry (UPLC/TQ-MS). Partial least squares - discriminant analysis (PLS-DA) score plots showed a clear separation between the PM10 exposed group and the control group. We observed the changes in endogenous metabolites related to neurotransmitter and amino acids including alanine, aspartate and glutamate metabolism and valine, leucine and isoleucine biosynthesis in PM10 exposed mice compared to control. Branched-chain amino acids (BCAA) were significantly upregulated in PM10 exposed group, indicating the alteration in BCAA metabolism.This study demonstrates that the LC-MS based-metabolic profiling can be used to understand the metabolism of PM10 exposed group on biological systems.

Oral Presentation : **ANAL2.O-16**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:00

Chair: Jongcheol Seo (POSTECH)

Structural and electrochemical studies of fluorine substituted $LiFe_{1-x}Mn_xBO_3$ as a cathode material for Li–ion battery

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Among the cathode materials of lithium-ion batteries, borate-based materials have been studied by many researchers due to their high theoretical capacity (220 mAh g^{-1}). $LiFeBO_3$ has good reversible capacity and safety with low open-circuit voltage (OCV). In previous studies, we have shown the improved discharge capacity by fluorine substitution in oxygen site of $LiFeBO_3$ but having structural instability. In this study, to increase structural stability, manganese has been applied to the iron site in F substituted $LiFeBO_3$ and $LiFe_{1-x}Mn_xBO_{3-\delta}F_{2\delta}$ (x = 0, 0.25, 0.5, 0.75, and 1.0), which have been synthesized by solid-state method and characterized their structure by X-ray diffraction (XRD). In order to verify the stability of the structure, an electrochemical performance test has also been performed by using the Galvano static charge-discharge measurements.

Oral Presentation : **ANAL2.O-17**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:04

Chair: Jongcheol Seo (POSTECH)

Quantitative Analysis of Anti-cancer Drugs and Its Fragmentation Pathways Using Ion Mobility Mass Spectrometry and Tandem Mass Spectrometry

Gyusub Yoon, Sooyeon Chae, MyungKook Son, Dongjoon Im, Dongvin Kwak, Da Gyeong Hyun, Chanju Won, Hugh I. Kim*

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Neuroblastoma is one of the representative childhood cancers and a highly heterogeneous disease affected by factors such as age at diagnosis, stage, and tumor biology. Multidrug regimen chemotherapy has been ongoing for high-risk patients and requires customizing to maximize treatment efficiency. To improve the outcomes for neuroblastoma, many research groups and institutes have developed precision medicine (personalized-medicine) using biochemical methods such as genomics and proteomics.Among them, pharmacogenomics and pharmacoproteomics are broader academic fields that identify genes or proteins involved in drug response or disease occurrence. Therefore, It is important to verify pharmacokinetics to develop pharmacogenomics and pharmacoproteomics.In this study, we establish a drug quantitation method for verifying pharmacokinetics using mass spectrometry. Quantitative analysis of Intracellular antidrug was performed using multiple reaction monitoring (MRM) analysis using RPLC-triple quadrupole mass spectrometry. For precise quantitative analysis, the mechanism of fragmentation used in MRM analysis was also investigated. Fragmentation pathways of anticancer drugs were identified using ion mobility mass spectrometry (IM-MS).

Oral Presentation : **ANAL2.O-18**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:08

Chair: Jongcheol Seo (POSTECH)

Purification of Non-Tagged Recombinant *α*-Synuclein Using Liquid Chromatography Based Separation Methods

Da Gyeong Hyun, Dongjoon Im, MyungKook Son, Sooyeon Chae, Dongvin Kwak, Chanju Won, Gyusub Yoon, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

α-Synuclein aggregates are the pathological hallmarks of synucleinopathies, including Parkinson’s disease and dementia with Lewy bodies. However, there is still no treatment for the synucleinopathies that has been established. To develop a therapeutic strategy, it is crucial to understand the molecular basis of *α*-synuclein aggregation and suppress the pathogenic amyloid aggregate formation. Up to date, as in-human studies are limited, the majority of research findings were based on *in vitro* experiments, with purified recombinant *α*-synuclein used to investigate self-assembly properties. Herein, we developed high-purity recombinant full-length *α*-synuclein expression and purification protocols without affinity tags or linkers. Furthermore, we performed a quality assessment of purified recombinant proteins to confirm the unique properties of *α*-synuclein via biophysical analyses including mass spectrometry-based identification, thioflavin T (ThT) fluorescence assay, and circular dichroism (CD). The compelling results imply that the proposed non-tagged *α*-synuclein preserves its biophysical properties, which can be used in further study to investigate the self-assembly property of *α*-synuclein.

Oral Presentation : **ANAL2.O-19**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:12

Chair: Jongcheol Seo (POSTECH)

Quantitative analysis of hydrogen isotopes in deuterium and hydrogen gases

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Gas Isotope Metrology team, Korea Research Institute of Standards and Science, Korea

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Stable isotopes of hydrogen include H and deuterium atom (D), and molecules include H_2 (Hydrogen), HD (Hydrogen Deuteride), and D_2 (deuterium). Recently, deuterium has been used instead of hydrogen in industries such as electronics and semiconductors. The diffusion velocity of deuterium is slower than ordinary hydrogen and can improve the stability of the industrial processes of products. Korea exploits more than half of the world market of deuterium and it all relies on import due to lack of industrial facilities to produce suitable deuterium. Many Korean companies are building deuterium production facilities to produce high-purity deuterium. The D_2 is produced by electrolysis of deuterium water (D_2O), the isotopes H_2 and HD exist as impurities with the deuterium gas produced in this process. Without regulation impurities affect the purity of deuterium gas and only high purity gas is required for industrial use. Therefore, determining impurities of D_2 is crucial. In this study, three high purity gases, H_2, D_2 and HD were used to analyze trace amounts of hydrogen isotopes using Precision Gas Mass Spectrometer (MAT271). Hydrogen isotopes present in each gas were quantified using sensitivity values of H_2, HD and D_2 gases. It has been confirmed that there are 300 μmol/mol of HD in H_2, 2500 μmol/mol of HD in D_2, and 5,000 μmol/mol of D_2 in HD. Further, planning to develop certified reference material (CRM) produced by high purity substances, which is for analyzing hydrogen isotopes and used as standard material to quantify the impurities of commercial D_2 gases.

Oral Presentation : **ANAL2.O-20**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:16

Chair: Jongcheol Seo (POSTECH)

Conformation Ensembles of Pathologically Disordered Proteins

Dongjoon Im, MyungKook Son, Da Gyeong Hyun, Sooyeon Chae, Chanju Won, Gyusub Yoon, Dongvin Kwak, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

As the number of people suffering from neurodegenerative diseases, such as dementia, grows, they have become a serious social burden. Nevertheless, the majority of dementia treatments aim to alleviate symptoms in the short term. Understanding the nature of a protein identified as a pathogen is required for developing a more effective treatment. However, intrinsically disordered proteins, which have been identified as the cause of dementia, can exist in a heterogeneous states and do not have a specific favorable structure, particularly at the early stage of aggregation. As a result, an analysis method capable of comprehensively analyzing various structure ensembles in which proteins may exist is required. Herein, we investigated the conformation ensemble of amyloid-β (1-42) and tau, which are closely related to the pathological hallmarks in Alzheimer's disease using replica exchange molecular dynamics simulations. We identified protein interactions that play an active role on the early stages of amyloid aggregation by *in silico* analyses. Furthermore, combined with an interdisciplinary biophysical approach, we observed how the theoretically identified structural properties were expressed *in vitro*. Overall, this methodology, based on the structural dynamics of pathologically disordered proteins, could be applied to theoretically predict and inhibit self-assembly properties.

Oral Presentation : **ANAL2.O-21**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:20

Chair: Jongcheol Seo (POSTECH)

The pharmaceutical and biomimetic models with quantitative analysis for precision medicine

Sooyeon Chae, Gyusub Yoon, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Precision medicine for solid cancer is targeted therapy based on scientific evidence such as pharmaceutic factor, gene, protein, and metabolite. Therefore, investigating accurate scientific evidence is critical for providing precision medicine for each patient. In general, scientific evidence was firstly investigated in the laboratory cell-based screening model. However, this model does not consider pharmacokinetics, structures, and microenvironments of solid cancer. Consequently, drugs efficacy or targeting biomarkers have shown discriminated results in clinical tests or therapy. Therefore, it is necessary to discover reliable biomarkers using pharmaceutical and biomimetic models at the pre-clinical level.Several clinical tests showed that the multidrug regimens have synergistic drug efficacy. However, the specific mechanisms of this effect and appropriate combinations of drugs are still ambiguous due to challenges at mimicry of pharmacokinetics and the tumor microenvironment at the laboratory level. We have constructed the pharmaceutical and biomimetic models with our Artificial Circulatory System for Tumoroid (ACST). Pharmacokinetic software, and microfluidic systems were used for the ACST systems. The results obtained from cutting-edge analysis techniques, including mass spectrometry (MS), ion mobility mass spectrometry (IM-MS), and spectroscopy, provided detailed drug action mechanisms based on the quantitative analyses.

Oral Presentation : **ANAL2.O-22**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:24

Chair: Jongcheol Seo (POSTECH)

Synthesis of Hollow mesoporous carbon spheres (HMCSs) incorporated with gold nanoclusters

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Electrochemiluminescence (ECL) is an electrochemical process in which species generated at electrodes undergo high energy electron transfer reactions to form excited states that emit light. Recent studies including ours demonstrated analytical benefits of Au nanoclusters as a stable and biocompatible ECL emitter. In this study, we synthesized hollow mesoporous carbon spheres (HMCSs) incorporating glutathione-stabilized Au nanoclusters (Au NCs) within mesoporous shell of HMCSs. We envision the HMCSs incorporating Au NCs as an efficient ECL emitter platform exhibiting amplified ECL of the Au NCs by confining the NCs within the conductive mesoporous shell of HMCSs.

Oral Presentation : **ANAL2.O-23**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:28

Chair: Jongcheol Seo (POSTECH)

Photoluminescence and electrochemiluminescence properties of Au(I)-glutathione complexes depending on pH conditions

Jeongyun Choi, Joohoon Kim*

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Electrochemiluminescence (ECL) is an electrochemical phenomenon in which electrochemically-generated species undergo electron transfer reactions to produce excited species emitting light at electrodes. The ECL has the advantages of high sensitivity and low background noise, and thus has been used in various fields such as biosensing, clinical diagnosis, environmental monitoring. In this study, we synthesized Au(I)-glutathione complexes under different pH conditions, then compared their ECL properties as well as photoluminescence (PL) properties. Glutathione is a tripeptide having two carboxyl groups and one amine group. As pH conditions change, Au(I)-glutathione complexes undergo a reversible assembly-disassembly process due to the functional groups of glutathione. Therefore, the aggregation extent of the Au(I)-glutathione complexes varies depending on the pH conditions. Because the aggregation of the Au(I)-glutathione complexes results in the aggregation-induced emission (AIE) of the complexes, we demonstrated different ECL and PL behaviors of the Au(I)-glutathione complexes depending on the pH conditions.

Oral Presentation : **ANAL2.O-24**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:32

Chair: Jongcheol Seo (POSTECH)

[Withdrawal] Condensation effect caused by phase change of insulin due to PEG

Dongvin Kwak, Hugh I. Kim[*], Sooyeon Chae, MyungKook Son, Dongjoon Im, Da Gyeong Hyun, Chanju Won, Gyusub Yoon

Department of Chemistry, Korea University, Korea

- Withdrawal -

Oral Presentation : **ANAL2.O-25**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:36

Chair: Jongcheol Seo (POSTECH)

Influence of plasma treatment on AuNRs immobilized on ITO surfaces

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Localized surface plasmon resonance (LSPR) is a unique property associated with certain metallic nanomaterials (e.g., Au, Ag, Cu). LSPR is a collective oscillation of conduction band free electrons in metallic nanostructures due to interactions with light. The LSPR spectrum of plasmonic nanoparticles (eg. Au, Ag, Cu) is influenced by the size, shape, composition, and change in dielectric properties of the surrounding medium (refractive index). Gold nanoparticles (AuNPs) have been considered in this work because of their broadly tunable size, shape, and structure-dependent optical properties, the easy possibility of surface modifications by biological and organic molecules, biocompatibility, and photostability. Plasma, the fourth state of matter, is a partially ionized gas consisting of electrons, ions, and neutral atoms/ molecules. Radiofrequency (RF) plasma, a nonthermal plasma (the gas temperature is as low as room temperature), is often used to remove surface capping material and to change the morphology of metallic nanoparticles (NPs). In this study, we discuss the spectral, structural, and electrochemical behavior of AuNRs immobilized of ITO for various plasma exposure times by dark-field (DF) microscopy and spectroscopy, scanning electron microscopy (SEM), and cyclic voltammetry (CV). Single gold nanorods (AuNRs) of considerable size were immobilized on the ITO surface and have been subjected to various plasma exposure times. We analyze here the LSPR linewidth variations of scattering spectra, effect in aspect ratio (AR) and morphology of AuNRs from SEM image analysis, and possible facet modification of AuNRs from CV analysis as a function of plasma exposure time.

Oral Presentation : **ANAL2.O-26**

Oral Presentation of Young Analytical Chemists II

Room 201 FRI 10:40

Chair: Jongcheol Seo (POSTECH)

Engineering Oxidase-Mimicking Activity of Dendrimer-Encapsulated Pt Nanoparticles

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Here, we report the engineered oxidase-mimetic activity of dendrimer-encapsulated Pt nanoparticles (Pt DENs) by precisely controlling their sizes in the diameter range of 1.8 – 3.1 nm. Using a dendrimer-template method, we synthesized five different Pt DENs (i.e., Pt_{200}, Pt_{220}, Pt_{550}, Pt_{880}, and Pt_{1320} DENs) having sizes in the range of 1.8 – 3.1 nm. The as-synthesized Pt DENs exhibit oxidase-mimetic activity for the oxidation of Amplex Red to form fluorescent resorufin in the presence of oxygen. Mechanistic study indicates that Pt DENs catalyzed activation of dissolved oxygen to generate reactive oxygen species (ROSs) (i.e., OH•, $O_2^{\bullet -}$, and $^1O_2$) and the ROSs are responsible for the oxidation of Amplex Red to resorufin. The enzyme-mimetic activity of Pt DEN was tunable by changing the size of Pt nanoparticles, and especially up to Pt_{1320} DENs with a diameter of 3.1 nm. The oxidase-like activity of Pt DENs tends to increase as their size increased. Interestingly, Pt_{1320} DENs exhibit a ~117-fold higher catalytic activity compared to Pt_{200} DENs, although they were only 1.2 nm larger in diameter than Pt_{200} DENs. We envision that this study can provide insights into the design of artificial enzymes having excellent performance.

Award Lecture in Division : **LIFE.O-8**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 10:35

Chair: Jiwon Seo (GIST)

Targeted Protein Upregulation via Modulation of Protein-Protein Interaction to Potentiate STING Agonist Immune Therapy

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Protein-protein interaction (PPI) plays a pivotal role in various biological systems and many complex diseases including cancer, neurodegenerative diseases, and metabolic diseases are often caused by aberrant PPIs. Given its significance in the biological systems, the identification of PPI modulators could be a starting point for drug discovery and chemical biology research. However, the high-throughput screening of conventional compound libraries hasn’t been successful, due to the different structural requirement of PPI modulators. Thus, there is a great demand in the construction of novel molecular diversity. Diversity-oriented synthesis (DOS) can provide a collection of diverse and complex drug-like small molecules, which is critical in the development of new chemical probes for biological research of undruggable targets. Modulating target proteins via the ubiquitin-proteasome system has recently broadened the scope of pharmacological inventions. Stimulator of interferon genes (STING) activation is a promising strategy for immuno-oncology that promotes systemic antitumor immunity at the interface of innate and adaptive immunity. However, from the current clinical investigations of STING agonists, dysregulated STING expression or poor STING agonist pharmacokinetics pose major challenges that limit the robust antitumor response. Herein, we propose UPPRIS (upregulation of target proteins by protein-protein interaction strategy) to overcome these limitations. We discovered that the small molecule SB24011 inhibits the STING–TRIM29 E3 ligase interaction, thereby blocking the TRIM29-mediated STING degradation. SB24011 enhanced the cGAMP-mediated immunity by upregulating cellular STING levels through blocking TRIM29-induced K48 linkage-specific ubiquitination. Thus, SB24011 potentiated the immuno-oncological efficacy of cGAMP and anti-PD-1 therapy for tumor regression, confirmed in CT26 and B16F10 syngeneic mouse models. Our work successfully demonstrated that targeted protein upregulation of STING is a promising strategy for cancer immunotherapy. Furthermore, UPPRIS could be utilized to comprehend the unexplored protein-protein interaction interfaces and advance our understanding of biological processes. Overall, we anticipate that UPPRIS, an opposite approach of PROTAC, brings breakthroughs in clinical and academic research fields.

Oral Presentation : **LIFE.O-1**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 09:00

Chair: Eunha Kim (Ajou University)

AmylScan: A web-based application to identify the hot sites in amyloid fibril formation

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Finding of the aggregation-prone regions of the proteins related to neurodegenerative diseases is very important for therapeutics purposes. The structural transitions of monomeric proteins is the first step toward forming the primary nuclei of β-sheets in the early stages of fibrillation process. The regions that open earlier in the monomeric structural transitions play the main role in starting the fibrillation. Therefore, it will be of critical importance to identify those hot sites that are responsible for the initiation of local deformation in a given the monomeric protein. In this paper, we present AmylScan, a free web-based application to predict the hot sites that have the potential to form fibril fragments. AmylScan uses a combination of sequence and structural analyses to predict the amyloidogenic regions in the proteins. From the hydrophobicity and β-structure propensity of each amino acid is used to identify the aggregation-prone sites. Then, targeted molecular dynamics (TMD) is performed to monitor local deformations and determines their priorities in the structural transition. AmylScan has a mutation option to model single or multiple mutated structures and compare their hydrophobicities and propensities with the native structure. We believe that AmylScan would be one of the useful applications for experimentalists who investigate the mechanism of the amyloid fibril formation.Availability and implementation: AmylScan is available from http://bioinf.modares.ac.ir/software/AmylScan/.

Oral Presentation : **LIFE.O-2**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 09:12

Chair: Eunha Kim (Ajou University)

Contagious aggregation: Transmittable protein aggregation in cellular communities initiated by synthetic cells

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The aggregation of amyloidogenic proteins causing neurodegenerative diseases has uncontrollable and transmittable characteristics which are often associated with lipid membranes in a highly complex physiological environment. Although several approaches using natural cells and micro droplets have been reported, comprehensive investigations focusing on the protein-membrane association are highly challenging, mostly because of the lack of proper molecular tools. Here, we report a new supramolecular approach using a synthetic cell system capable of controlling the initiation of protein aggregation and mimicking various conditions of lipid membranes, thereby enabling systematic investigations of membrane-dependent effects on protein aggregation. By concurrent use of the protocells with live cells, this approach clearly visualized the inter- and intracellular trajectories of the contagious aggregation of proteins associated with lipid membranes from the initiation to the end of the process. Thus, our approach demonstrated a new pathway to construct a new type of protocell as a research platform for systematic investigations of biological processes and provides a step towards interrogating the pathological implications of membrane-associated contagious aggregation of amyloidogenic proteins in several natural systems.

Oral Presentation : **LIFE.O-3**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 09:24

Chair: Eunha Kim (Ajou University)

A combinatorial strategy for identification of spatial proteins at membrane contact sites

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Cellular organelles communicate with one another to regulate a variety of vital cellular processes including biomolecule exchanges, homeostasis and signaling. Since organelle communications are largely mediated by proteins at membrane contact sites (MCS), identification of the proteins at MCS is crucial to understand functions and mechanism of organelle communications. In this context, selective enrichment of target proteins using streptavidin-biotin binding pair system with a combination of proximal biotin labeling techniques using engineered ascorbate peroxidase (APEX) and promiscuous biotin ligase (pBirA / TurboID) have been exploited intensively. However, for reliable, accurate and precise protein identification, more selective and efficient enrichment of target proteins at MCS is highly required. Recently, our group has demonstrated a novel synthetic binding pair system such as cucurbit[7]uril-adamantylammonium (Ad) and its application for APEX-mediated chemical labelling to proximal proteins with Ad and its selective visualization using CB[7]-dye. This synthetic pair works similarly in binding to streptavidin-biotin, but its binding is orthogonal to that of streptavidin-biotin.In this presentation, we will discuss development of a new proteomic tool by a combination of both orthogonal binding pair systems (CB[7]-Ad, streptavidin-biotin) with two different proximity labeling enzymes (APEX2 and TurboID), as well as its use for

identification of the proteins at mitochondria-associated endoplasmic reticulum membranes (MAM) where mitochondria and ER, both organelles are facing each other.

Oral Presentation : **LIFE.O-4**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 09:36

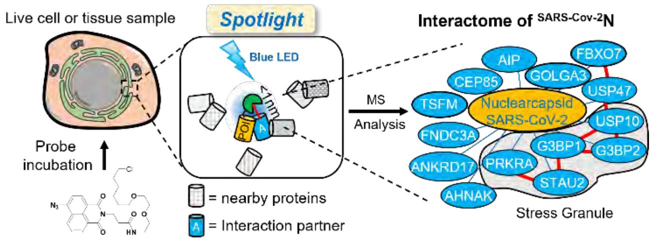
Chair: Eunha Kim (Ajou University)

Spatiotemporal protein crosslinking by light activation (Spotlight) for in-vivo interactome mapping

Pratyush Mishra[*], **Hyun-Woo Rhee**[1,*]

Department of Chemistry, Seoul national universuty, Korea
[1]*Department of Chemistry, Seoul National University, Korea*

To identify the interactome of POI in live cells, Among the various chemical labeling and chemical crosslinking methods which have been combined with mass spectroscopy, photo-crosslinking method have provided in vivo protein-protein interaction partner in live cells with less perturbation to the cellular physiology. However it is still very hard to genetically introduce photo-reactive groups to the POI. Furthermore, many photo-crosslinkers are designed to be activated by ultraviolet (UV) light which causes photo-toxicity and suffers from low tissue penetration. Herein, we developed a visible light activable fluorescent photo-crosslinking ligand which can be genetically introduced to the POI-conjugated HaloTag. Its ability to crosslink physically interacting proteins was confirmed by covalently capturing a rapamycin-induced protein interaction between FK506 binding protein (FKBP) and the FK506-rapamycin binding (FRB) domain in living cells under the presence of rapamycin , probe and visible light activation. Our method successfully captures stress induced proteome change as well as enables photocrosslinking in tissue samples. Since our method is orthogonal to current proximity labeling methods, we also confirmed that our method can be compatibly utilized with TurboID (Spotlight-Turbo). Using Spotlight, we attempt to identify the host interactome of Nucleocapsid (N) protein of SARS-CoV-2, which is essential for viral genome assembly process. From the mass analysis of the VL1-crosslinked product of N-HaloTag in HEK293T cells, RNA binding proteins in stress granule and P-body proteins were enriched in the crosslinked samples. From follow-up study, we confirmed that our method can reveal the specific interactome of N protein within a few angstrom distance in live cells


Live cell or tissue sample
Spotlight
Blue LED
Interactome of $^{SARS\text{-}Cov\text{-}2}N$
MS
Analysis
Probe
incubation
POI
A
= nearby proteins
A = Interaction partner
AIP
FBXO7
CEP85
GOLGA3
USP47
TSFM
Nuclearcapsid
SARS-CoV-2
USP10
FNDC3A
G3BP1
G3BP2
ANKRD17
PRKRA
STAU2
AHNAK
Stress Granule

Oral Presentation : **LIFE.O-5**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 09:48

Chair: Eunha Kim (Ajou University)

Oxidative post-translational modification by exogenous reactive oxygen species as chemical leverage for regulating autophagy

Mingyu Park, Tae-Hyuk Kwon[1,*], Taiho Park[2,*], Duyoung Min[1,*], Taehyun Kim[2], Chaiheon Lee[3]

Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*
[2]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*
[3]*Chemistry, Ulsan National Institute of Science and Technology, Korea*

Autophagy modulation is attracting attention as a promising target for enhancing cancer therapy. Reactive oxygen species (ROS) are key physiological factors that control autophagic flux, although their therapeutic mechanism of action and regulation have remained unclear. Herein, we report oxidative post-translational modification (oxPTM) as chemical leverage for autophagy modulation. Using photoactivatable Ir(III) complex B2, which spatiotemporally oxidises lysosomes and perturbs autophagic flux, we identified significant oxPTM of amino acid residues (Met, Arg, or Lys) in proteins required for lipogenesis and membrane fusion. In vitro experiments clarified the effect of oxPTM on cellular functions involved in autophagy. Our analyses unprecedentedly revealed that chemical oxPTM of regulatory proteins can modulate autophagy along with direct lipid membrane peroxidation, resulting in effective cancer cell death. This study is expected to inspire chemically amenable therapies based on oxPTM.

Oral Presentation : **LIFE.O-6**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 10:00

Chair: Eunha Kim (Ajou University)

Development of combination therapy for STING agonist elevating immune response

Hee Ra Jung, Sanghee Lee[1,*], Eunha Kim[2,*]

Creative Research Center for Brain Science, Korea Institute of Science and Technology, Korea
[1]*Neuromedicin department, Korea Institute of Science and Technology, Korea*
[2]*Department of Molecular Science and Technology, Ajou University, Korea*

STING (Stimulator of interferon genes) has been emerged as a key mediator in the next generation of cancer immunotherapy to replace tumor immunophenotype from ‘cold’ to ‘hot’ by stimulation of innate immunity. The natural ligand for STING, such as 2’3’-cyclic GMP-AMP(cGAMP), or synthetic cyclic di-nucleotide (CDN) type of STING agonists activate IFN-mediated immune response and promote anti-cancer immunity. Despite the promising pre-clinical outcome, synthetic CDNs are limited in clinics due to the narrow application via IT administration and unfavorable pharmacokinetic properties. Therefore, there exists continuous effort to develop a combination therapy with synergistic effects for STING agonists. Here, we report a new compound for a STING activator that enhanced cGAMP-induced type I IFN innate immune response by stabilizing the STING-TBK1-IRF3 (Interferon regulatory transcription factor 3) complex. This potential compound strengthens activation of STING, TBK1, and IRF3 and the phosphorylated IRF3 dimer then enhances the expression of type I IFN. Furthermore, it exerts an anti-cancer effect in the syngeneic mouse model by suppressing tumor size. It could be a novel candidate for cancer immunotherapy drugs overcoming the limitations of existing administration approaches.

Oral Presentation : **LIFE.O-7**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 203 THU 10:12

Chair: Eunha Kim (Ajou University)

Point-of-care-test method for measurement of hydrogen sulfide level in blood

Yecheol Bak, Sehoon Kim[1,*]

Center for theragnosis, Korea Institute of Science and Technology/Program in Applied Bioengineering, Korea

[1]*Center for theragnosis, Korea Institute of Science and Technology, Korea*

Hydrogen sulfide (H_2S) is a 3rd gas transmitter that plays a role as an antioxidant and cell-signaling molecule in the body. Numerous researchers have been reported a decrease of H_2S level has been linked to several diseases such as Alzheimer's disease, hypertension, and diabetes. Traditional methods like HPLC, gas chromatography, and colorimetric-based assay have been used to detect H2S. However, these methods required high-cost equipment and a complex pre-treatment process which is hard to adapt in POCT.In our case, we have developed a protein-free one-step method that is practical for applying to a portable POCT method and highly selective metal complex toward H_2S using the electrochemiluminescence (ECL) technique. Without any further pretreatment, we have successfully been measured a difference between the disease group and control group's H_2S blood level in an animal model.

Oral Presentation : **ORGN.O-1**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 09:00

Chair: Sunggi Lee (DGIST)

Pd-Catalyzed Cross Coupling Reaction of Heteroarylsilver Intermediate Generated via Intramolecular Oxyargentation of Benzyne

Young-Kyo Jeon, Won-SuK Kim[1,*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea

[1] *Chemistry Department of Nano-Science, Ewha Womans University, Korea*

Benzoxazoles are appealing moieties in widespread fields including pharmaceuticals and fluorescent materials. Herein, we reported Pd-catalyzed cross coupling reaction of benzoxazolylsilver intermediates for the synthesis of benzoxazole derivatives. The unprecedented key benzoxazolylsilver intermediate is formed by silver fluoride mediated intramolecular oxyargentation of amidoaryne precursors. Subsequent Pd-catalyzed coupling reactions of aryl iodides with an in situ generated silver intermediate allowed facile access to valuable C7-arylated benzoxazole derivatives with broad functional group tolerance and substrate scope. Mechanistic studies have shown that controlling the timing between benzyne formation/oxy-argentation and transmetalation is a significant factor in the reaction system. Notably, it was found that the position of silyl group is important for benzyne formation because C-Si bond cleavage by AgF is affected by possibility of 1,5-Brook rearrangement and C-Si bond strength depending on the position of the silyl group.

Oral Presentation : **ORGN.O-2**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 09:10

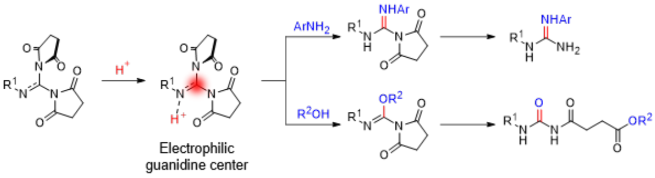
Chair: Sunggi Lee (DGIST)

Utilization of the Guanidine Carbon Center as a Carbon Electrophile by Guanidine Cyclic Diimide Formation

Taeyang An, Yan Lee*

Department of Chemistry, Seoul National University, Korea

AbstractThe guanidine carbon center can be electrophilic considering that it is connected to three electronegative nitrogen atoms. However, nucleophilic reactions at the guanidine carbon center are relatively underdeveloped because the resonance-stabilized ground state of the guanidine group reduces the electrophilicity of the carbon center. Herein, we propose a versatile guanidine C–N bond substitution strategy entailing the formation of guanidine cyclic diimide (GCDI) structures, which effectively destabilize the resonance structure and enhance the electrophilicity of the guanidine carbon center. In the presence of acid additives, the guanidine carbon center of GCDIs undergoes nucleophilic substitution reactions with various amine and alcohol nucleophiles to provide N,N'-disubstituted guanidines and N-acylurea products, respectively. GCDI-based nucleophilic substitution reactions can be conducted under mild, metal-free reaction conditions, and exhibit good functional group tolerance.References1. An, T.; Kang, B.; Kang, S.; Pac, J.; Youk, J.; Lin, D.; Lee, Y. Guanidine cyclic diimides and their polymers. Chem. Commun. 2019, 55, 10222–10225.2. An, T.; Lee, Y. Nucleophilic Substitution at the Guanidine Carbon Center via Guanidine Cyclic Diimide Activation. Org. Lett. 2021, 23, 9163–9167.



Oral Presentation : **ORGN.O-3**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 09:20

Chair: Sunggi Lee (DGIST)

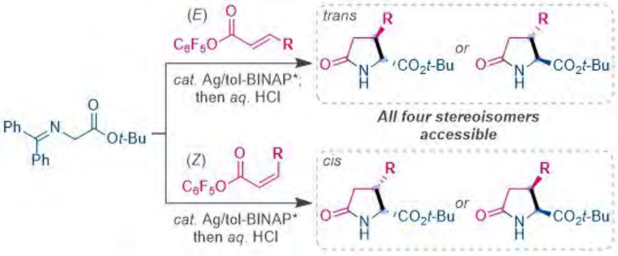
Enantio- and Diastereodivergent Silver-Catalyzed Synthesis of Chiral Pyroglutamic Acid Esters

Byungjun Kim, Sarah Yunmi Lee[1,*]

chemistry, Yonsei University, Korea

[1]*Department of Chemistry, Yonsei University, Korea*

Despite remarkable advances in the field of asymmetric catalysis, simultaneous control of both relative and absolute configurations of multiple stereogenic centers remains a considerable challenge. Recently, enantio- and diastereodivergent processes have attracted great attention because it could permit selective access to any given stereoisomers of enantioenriched compounds with multiple stereocenters. Herein, we present the silver-catalyzed method for the stereodivergent synthesis of chiral pyroglutamic acid esters via stereospecific 1,4-addition between glycine imine esters and β-substituted α,β-unsaturated perfluorophenyl esters followed by intramolecular lactamizations. By altering the combination of catalyst enantiomers (*R* or *S*) and the alkene geometry (*E* or *Z*), the full set of stereoisomers of the products with two vicinal stereocenters can be selectively obatined. This process allows access to an array of di- or trisubstituted pyroglutamic acid esters, including those containing an all-carbon quaternary stereocenter, with high diastereo- and enantioselectivity. The products generated from this method can be readily transformed into valuable chiral α-amino acid derivatives



Oral Presentation : **ORGN.O-4**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 09:30

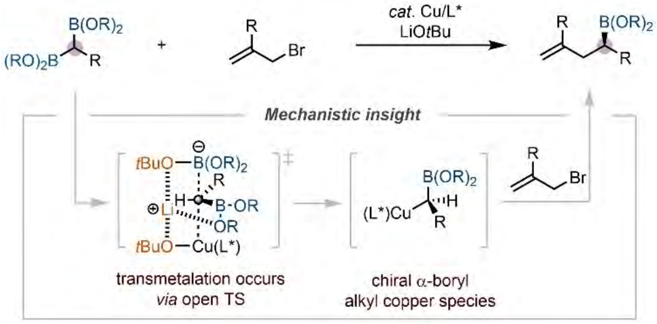
Chair: Sunggi Lee (DGIST)

Copper-Catalyzed Enantiotopic-Group-Selective Allylation of *gem*-Diborylalkanes

MinJae Kim, Seung Hwan Cho*

Department of Chemistry, Pohang University of Science and Technology, Korea

The development of an efficient catalytic reaction for preparing enantioenriched organoboron compounds received considerable attention over the past decades because they can serve as versatile intermediates in the synthesis of a range of natural products and pharmaceuticals. Herein, we report a copper-catalyzed enatiotopic-group-selective allylation of *gem*-diborylalkanes with allyl bromides. The combination of copper(I) bromide and H8-BINOL derived phosphoramidite ligand proved to be the most effective catalytic system to provide various enantioenriched homoallylic boronate esters, containing a boron-substituted stereogenic center that is solely derived from *gem*-diborylalkanes, in good yields with high enantiomeric ratios under mild conditions. Experimental and theoretical studies have been conducted to elucidate the reaction mechanism, revealing how the enatiotopic-group-selective transmetalation of *gem*-diborylalkanes with chiral copper complex occurs to generate chiral α-borylalkyl copper species for the first time. Additional synthetic applications to the synthesis of various chiral building blocks are also included.



Oral Presentation : **ORGN.O-5**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 09:40

Chair: Sunggi Lee (DGIST)

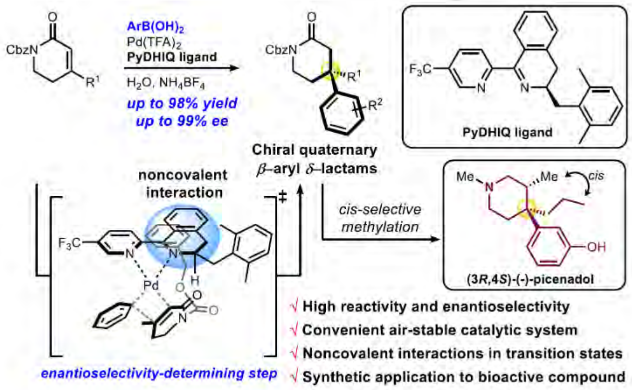
Highly Enantioselective Synthesis of β-Quaternary δ-Lactams by Palladium Catalysis Featuring Attractive Noncovalent Interactions: Asymmetric Synthesis of (-)-Picenadol

Doohyun Baek, Sukwon Hong[1,*]

Department of chemistry, Gwangju Institute of Science and Technology, Korea

[1]Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Herein, we report the first example of highly enantioselective conjugate addition of arylboronic acids to β-substituted α,β-unsaturated δ-lactams using Pd(II)/Pyridine-Dihydroisoquinoline (PyDHIQ) catalytic system, affording chiral δ-lactams bearing an all-carbon β-quaternary stereogenic center. The reaction proceeds under mild conditions employing water as a solvent and tolerates various arylboronic acids. The developed methodology was successfully applied to the first asymmetric formal synthesis of (-)-picenadol. In addition, it was disclosed that the unique skeleton of the PyDHIQ ligand plays a key role in providing attractive noncovalent interactions in an enantioselectivity-determining step based on DFT calculation and NCI plot.



Oral Presentation : **ORGN.O-6**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 09:50

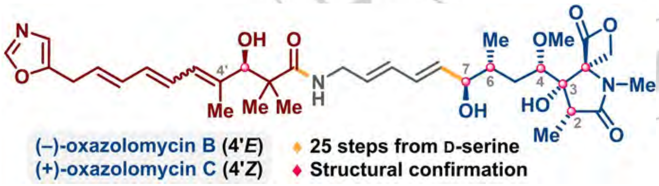
Chair: Sunggi Lee (DGIST)

Total Synthesis of Oxazolomycins B and C Using a Minimum Number of Chiral Sources

Yeonghun Song, **Sanghee Kim***

College of Pharmacy, Seoul National University, Korea

Oxazolomycins are a structurally and biologically interesting natural product family characterized by multi-conjugated systems along with lactam-lactone bicyclic-fused subunits. Herein, we report our efforts towards the first total synthesis of (−)-oxazolomycin B and (+)-oxazolomycin C from the intermediate of our previous synthesis of (+)-neoxazolomycin. The efficiency of our approach is derived from silicon-based reactions such as silyl triflate-mediated reductive oxazolidine ring-opening and Fürstner's Ru-catalyzed hydrosilylation and protodesilylation reactions. The total syntheses were achieved in a longest linear sequence of 25 steps from the amino acid serine in 3.6 and 2.7% overall yields, respectively. By analysis and comparison of spectral data, we confirmed the alleged structures of oxazolomycins B and C are correct.



Oral Presentation : **ORGN.O-7**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 10:00

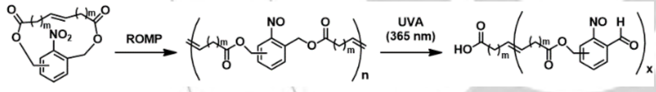
Chair: Sunggi Lee (DGIST)

Development of New Photo-Cleavable Polymers via ROMP

Bon Woo Koo, Dayong Song, Jae Woo Park*, Min Kim*, Cheoljae Kim*

Department of Chemistry, Chungbuk National University, Korea

New photo-cleavable polymers via ring-opening metathesis polymerization (ROMP) have been developed. By using well-known photo-cleavable functionality, *ortho*-nitrobenzyl esters, regioisomeric monomers were synthesized with ring sizes. Polymerizations were successfully demonstrated with Grubbs 2nd generation in 30 minutes, and degradations were also occurred under UVA irradiation within 1 hour.



Oral Presentation : **ORGN.O-8**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 10:10

Chair: Sunggi Lee (DGIST)

Remotely Controllable Supramolecular Rotor Mounted inside a Porphyrinic Cage

Avinash Dhamija, Kimoon Kim[1,*]

Center for Self-assembly and Complexity, IBS, India
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Biological machines such as adenosine triphosphate (ATP) synthase operate within specific nanoscopic domains inside the cellular matrix, which is the very basis for their remarkable precision and programmed mechanical motion of their constituent components and associated functions. The rotatory motion of the enzyme subunits is remotely controlled by chemical processes, such as proton (or Na^+) flux or ATP hydrolysis. Inspired by such natural systems, we have constructed a supramolecular rotor inside a nanostructured Zn-metallated porphyrinic cage by encapsulation of a tetrazine-based linear axle (LA) via metal-ligand coordination bond, followed by post-assembly modification to append a controllable side arm to LA via inverse electron demand Diels-Alder (IEDDA) reaction. While the rotor alone shows very slow or no motion, the addition of pyridine derivatives as a zinc coordinating ligand resulted in both 90° jump-like rotary motion and slow tumbling motion of the rotor in a stochastic manner. A reversible control over the dual motions of the rotor was achieved by the UV and visible light-induced coordination and dissociation of an azopyridine based ligand with Zn-centers as a signal transducer. The concept of confining molecular machines inside a molecular cage and remotely controlling their functions is beneficial not only for understanding the operation of biological machines but also for the development of functional nanoscale units for the controlled manipulation (via catalysis) and transportation of other chemical species (such as ions) through their 3D nanocavities.[1]ReferenceDhamija, A.; Das, C. K.; Ko, Y. H.; Kim, Y.; Mukhopadhyay, R. D.; Gunnam, A.; Yu, X.; Hwang, I-C.; Schäfer, L. V.; Kim, K. Chem 2022, 8, 543-556.

Oral Presentation : **ORGN.O-9**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 10:20

Chair: Sunggi Lee (DGIST)

Precisely controlled iSDT by activatable sonosensitizer combined with immune stimulant imiquimod

Subin Son, Ji Hyeon Kim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Sonodynamic therapy (SDT) is one of the promising cancer treatments due to its high tissue penetration ability. However, under ultrasound irradiation (US), US induces ROS generation in the undesired regions, which might show an off-target effect. To achieve selective toxicity in tumors without any toxicity in normal tissue, the development of the activatable sonosensitizer is necessary in the tumor microenvironment. Moreover, by combining immune adjuvant, a disadvantage of SDT can be overcome. We developed a methylene blue and imiquimod conjugated iSDT system (MB-R837). Under tumor microenvironment, sonosensitizer and immune adjuvant are released. In tumor-bearing mouse models, treatment of the iSDT platform with an immune checkpoint blockade inhibitor (α-PD-L1) resulted in an additional efficient immune response and memory function in terms of immunotherapy.

Oral Presentation : **ORGN.O-10**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 10:30

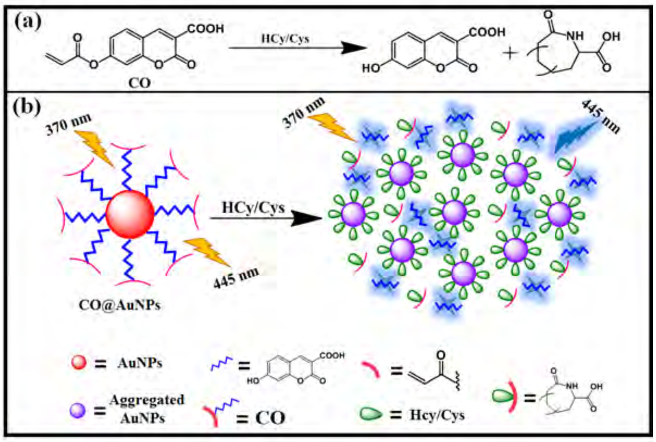
Chair: Sunggi Lee (DGIST)

Detection Time Based Selective Discrimination Of HCy From Cys Using Gold Nanoparticle Based Optical Probe And Its Application In Blood Plasma And Urine

Ratish Nair, Su Jin Na, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Hyperhomocysteinemia (a clinical condition with increased homocysteine (Hcy) in human blood) is associated with various acute health disorders. Selective discrimination of HCy from Cys is very important. Consequently, Hcy measurement in human plasma is essential for clinical management of several vascular, cardiac, renal, and age related pathologies. Rapid detection of plasma Hcy by simple optical technique would be beneficial for clinical purpose. Moreover, sensitivity at physiological condition, cost of the reagents, and obligatory requirement of non-aqueous media have carried limitation to this endeavor. In the current work, synthesis and characterization of a new Hcy selective nanoparticle probe CO@AuNPs is reported. CO@AuNPs showed remarkable colorimetric and fluorimetric properties with Hcy in 100 % aqueous medium at physiological as well as at variable pH. The probe CO@AuNPs, discriminates HCy from Cys using detection time. The biosensor CO@AuNPs, with lower detection limit (LOD) of 120 nM can also be utilized for colorimetric detection of HCy in biological samples. Being non-toxic and permeable in nature, CO@AuNPs can function as a colorimetric staining reagent for HCy in biological samples. CO@AuNPs were validated for detection of HCy using HPLC technique. The probe CO@AuNPs can be used for detecting HCy in blood plasma and urine.


(a)
COOH
CO
HCy/Cys
COOH
HO
NH
OH
(b)
370 nm
445 nm
HCy/Cys
370 nm
445 nm
CO@AuNPs
= AuNPs
= Aggregated AuNPs
COOH
HO
= CO
= Hcy/Cys
NH
OH

Oral Presentation : **ORGN.O-11**

Oral Presentations for Young Scholars in Organic Division

Tamna Hall A THU 10:40

Chair: Sunggi Lee (DGIST)

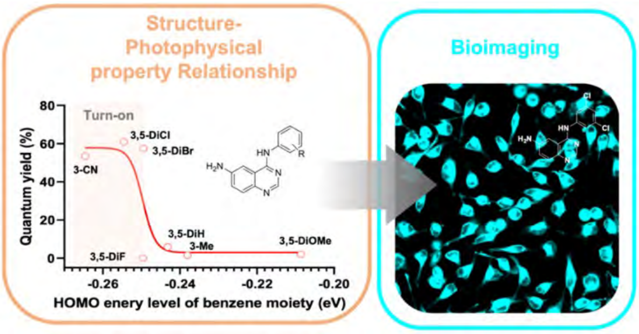
Development of N4-Phenyl quinazoline-4,6-diamine as a fluorophore and its application for the formaldehyde detection and cellular bioimaging

Jaeseok Lee, Jongmin Park*, Eunha Kim[1,*]

Department of Chemistry, Kangwon National University, Korea

[1]*Department of Molecular Science and Technology, Ajou University, Korea*

Fluorescent molecules has been used for various applications in biological system monitoring. Considering the complexity of cellular system, there is a huge demand for diverse fluorescent organic molecular scaffolds. We serendipitously discovered N4-Phenyl quinazoline-4,6-diamine as a fluorescent scaffold with turn-on characteristics. To improve the photophysical property of the initial fluorescence molecule, we synthesized the derivative of the N4-Phenyl quinazoline-4,6-diamine and found systematic correlation between electronic density of phenyl substituent of the scaffold and fluorescence intensity. By considering quantum yield and cellular uptake ability, we choose N4-dichlorophenyl quinazoline-4,6-diamine as a potential fluorophore for various biological applications. As a proof of concept, we developed formaldehyde (FA) fluorescent sensor by tailoring amine on 6-position of N4-dichlorophenyl quinazoline-4,6-diamine to employ 2-aza-cope rearrangement as the molecular detection mechanism with excellent turn-on ratio. The detection mechanism of the probe affords high specificity and sensitivity with observed limit of detection was approximately 100 nM. Finally, FA level in live HeLa cells were successfully visualized with the probe, exhibiting that N4-dichlorophenyl quinazoline-4,6-diamine can serve as a useful molecular scaffold for offering various fluorescent sensors toward the investigation of physiological and pathological process in live cells.


Structure-
Photophysical
property Relationship
Bioimaging
Turn-on
Quantum yield (%)
80
60
40
20
0
3,5-DiCl
3,5-DiBr
3-CN
3,5-DiH
3-Me
3,5-DiOMe
3,5-DiF
-0.26
-0.24
-0.22
-0.20
HOMO enery level of benzene moiety (eV)
HN
R
H_2N
N
Cl
Cl
HN
H_2N
N

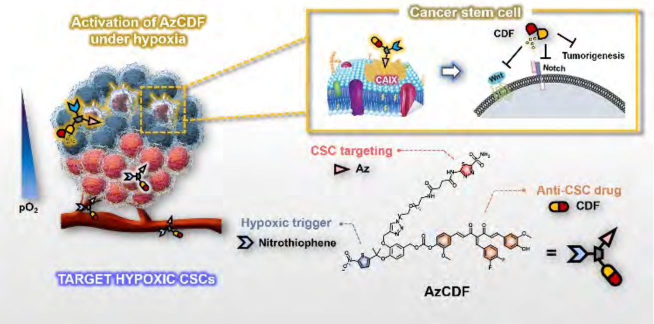
Oral Presentation : **ORGN.O-12**
Oral Presentations for Young Scholars in Organic Division
Tamna Hall A THU 10:50
Chair: Sunggi Lee (DGIST)

Designing a Small Molecule for Targeting Hypoxic Cancer Stem Cells

Ji Hyeon Kim, Miae Won[1], Jongseung Kim[*]

Department of Chemistry, Korea University, Korea
[1]*R&D institute, TheranoChem Inc., Korea*

Breast cancer consists of heterogenic subpopulations, which determine the prognosis and response to chemotherapy. Among these subpopulations, a very limited number of cancer cells are particularly problematic. These cells, known as breast cancer stem cells (BCSCs), are thought responsible for metastasis and recurrence. They are thus major contributor to the unfavorable outcomes seen for many breast cancer patients. BCSCs are more prevalent in the hypoxic niche. This is an oxy-gen-deprived environment that is considered crucial to their proliferation, stemness, and self-renewal, but also one that makes BCSCs highly refractory to traditional chemotherapeutic regimens. Here we report a small molecule construct, AzCDF, that allows the therapeutic targeting of BCSCs and which is effective in normally refractory hypoxic tumor environments. A related system, AzNap, has been developed that permits CSC imaging. Several design elements are incorporated into AzCDF, including the CAIX inhibitor, acetazolamide (Az) to promote localization in MDA-MB-231 CSCs, a di-methylnitrothiophene subunit as a hypoxia trigger, and a 3,4-difluorobenzylidene curcumin (CDF) as a readily released therapeutic payload. This allows AzCDF to serve as a hypoxia-liable molecular platform that targets BCSCs selectively that decreases CSC migration, retards tumor growth and lowers tumorigenesis rates as evidenced by a combination of in vitro and in vivo studies. To the best of our knowledge, this is the first time a CSC-targeting small molecule has been shown to prevent tumorigenesis in an animal model.


Activation of AzCDF under hypoxia
Cancer stem cell
CAIX
CDF
Tumorigenesis
Wnt
Notch
pO2
CSC targeting
Az
Anti-CSC drug
CDF
Hypoxic trigger
Nitrothiophene
AzCDF
=
TARGET HYPOXIC CSCs

Oral Presentation : **MEDI.O-1**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 09:00

Chair: Kwan-Young Jung (KRICT)

Investigation of benzimidazole anthelmintics as an oral anticancer agent

Jiyoon Jang, Kwangho Lee[1,*], Byumseok Koh[1,*]

Korea Research Institute of Chemical Technology & Sungkyunkwan University, Korea
[1]*Korea Research Institute of Chemical Technology, Korea*

Benzimidazole anthelmintic drugs, including fenbendazole, mebendazole, nocodazole, and oxibendazole, are widely used in dogs and humans to treat parasitic worm infections. Recently, there has been social controversy regarding whether these benzimidazole anthelmintic drugs can be used as anticancer drugs. For decades, articles on the anticancer effect of benzimidazole anthelmintic drugs have been reported. Studies have suggested that benzimidazole anthelmintic drugs inhibit microtubule dynamics, which play a crucial role in mitosis, cell division and cell structure maintenance, by promoting microtubule depolymerization. However, there is still no conclusive evidence of whether these benzimidazoles can be used for anticancer treatment. Therefore, we explored the anticancer efficacy of benzimidazole anthelmintic drugs in vitro and their mechanism of action. We also conducted pharmacokinetic studies of two benzimidazole anthelmintics and assessed the predictive systemic efficacy. Finally, we present the anticancer efficacy of benzimidazole anthelmintics' putative metabolites from hydrolysis. In this presentation, benzimidazole anthelmintics' antitumor mechanism of action, drug-like properties and potential use for anticancer treatment will be discussed based on our research.

Oral Presentation : **MEDI.O-2**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 09:10

Chair: Kwan-Young Jung (KRICT)

Design, synthesis, and biological evaluation of thiazolidinedione-based HDAC6 inhibitors to overcome methamphetamine addiction

Sonam Jha

PHARMACY, Keimyung University, Korea

Thiazolidinedione is a five-membered heterocycle that is widely used in drug discovery endeavors. In this study, we report the design, synthesis, and biological evaluation of a seriesof thiazolidinedione-based HDAC6 inhibitors. In particular, compound 6b exerts an excellent inhibitory activity against HDAC6 with an IC50 value of 21 nM, displaying a good HDAC6selectivity over HDAC1. Compound 6b dose-dependently induces the acetylation level of alpha-tubulin via inhibition of HDAC6 in human neuroblastoma SH-SY5Y cell line. Moreover, compound 6b efficiently reverses methamphetamine-induced morphology changes of SH-SY5Y cells via regulating acetylation landscape of alpha-tubulin. Collectively, compound 6b represents a novel HDAC6-isoform selective inhibitor and demonstrates promising therapeutic potential for the treatment of methamphetamine addiction.Keywords: HDAC6 inhibitors; thiazolidinedione; methamphetamine; drug addiction

Oral Presentation : **MEDI.O-3**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 09:20

Chair: Kwan-Young Jung (KRICT)

Oxazole analogs as novel interleukin-33 inhibitors

Geonhee Jang, Eunji Kim[1], Sang-Hyun Son[1], Youngjoo Byun[*], Youngjoo Byun[*]

Department of Pharmacy, Korea University, Korea

[1]*Azcurin Inc., Korea*

Interleukin-33 (IL-33) is an epithelial-derived cytokine that plays an important role in allergic immune diseases such as asthma and atopic dermatitis. IL-33 binds to the IL-33-specific primary receptor ST2 to form a heterodimeric complex, which then forms a triple complex with the IL-1R accessory protein. Although IL-33 is considered an attractive target for the treatment of allergy-related diseases, only a few small molecules have been reported to date. We designed and synthesized over 40 oxazole analogs to inhibit the interaction between IL-33 and ST2. Oxazole analogs were synthesized via 3 or 4 synthetic steps using ethyl 2-aminooxazole-4-carboxylate as the starting material. The Sandmeyer reaction, the palladium-catalyzed Suzuki reaction, and the Heck reaction were used to prepare the core scaffold. The final compounds were evaluated using an in vitro ELISA assay, a cell-based assay, and a cell toxicity assay using HepG2 cells. According to the structure-activity relationship (SAR) studies, the electron-donating groups of the phenyl ring substituted at the 5-position in oxazole ring increased the IL-33-inhibitory activities as compared to the electron-withdrawing groups. In addition, the electron-donating substituent at the m-position was more potent than that at the p-position. Among the synthesized compounds, KB-2728 with -SCH3 group at m-position showed an IC50 value of 4.6 nM in an ELISA assay with no cell toxicity to 30 μM in a HepG2-based cell cytotoxicity study. KB-2718 can be utilized as a hit compound for further structural modifications of oxazole-based IL-33 inhibitors.Keywords : Interleukin-33, oxazole, ELISA, SAR

Oral Presentation : **MEDI.O-4**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 09:30

Chair: Kwan-Young Jung (KRICT)

Design of pH-Responsive Nano-Transfersomes for Enhanced Photodynamic Therapy

Soo Ho Yeo

Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea

Photodynamic therapy (PDT) is a non-invasive and tumour-specific therapy. Photosensitizers (PSs) (essential ingredients in PDT) aggregate easily owing to their lipophilic properties. The aim of this study was to synthesise a PS and design a biocompatible lipid-based nanocarrier to improve its bioavailability and pharmacological effects. PS-loaded nano-transfersomes were fabricated by sonication. The characteristics of synthesised PS and nano-transfersomes were assessed. The effects of PDT were evaluated by 1,3-diphenylisobenzofuran assay and by measuring photo-cytotoxicity against HeLa and A549 cell lines. I would like to briefly introduce recent approaches for photosensitiser-loaded nano-transfersomes and related applications.

Oral Presentation : **MEDI.O-5**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 09:40

Chair: Kwan-Young Jung (KRICT)

Development of Therapeutic Agent against SARS-CoV-2 through Drug Repositioning

Yeonju Shin, Seonggon Kim[1], Berehe Solomon Girmay[1], Chang-Soo Yun[1], Sikwang Seong[1], Dong-Su Kim[1], Soo Bong Han[1,*]

Department of Pharmacy/Infectious Diseases Therapeutic Research Center , Chungbuk Natioanl University/Korea Research Institute of Chemical Technology , Korea

[1]*Infectious Diseases Therapeutic Research Center, Korea Research Institute of Chemical Technology, Korea*

At the end of 2019, a new type of coronavirus, designated SARS-CoV-2, has emerged and caused an outbreak of abnormal viral pneumonia. This novel coronavirus has spread rapidly and has made the entire world a pandemic. In spite of growing the confirmed case, effective treating agent against SARS-CoV-2 was not existed at the early stage of pandemic. In this regard, our research group started to develop antiviral drug employing drug repositioning strategy. This strategy is one of the fastest routes for discovering antiviral drug. As a result, the key compound, KCO011, was discovered through high-throughput screening of 1,500 FDA-approved drugs. In vitro CPE and image-based assays showed that KCO011 exhibited 5-fold better activity than remdesivir. Evaluation of in vitro ADME and in vivo PK of KCO011 showed moderate profiles. Further studies on our promissing drug candate, KCO011, are currently underway.

Oral Presentation : **MEDI.O-6**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 09:50

Chair: Kwan-Young Jung (KRICT)

Design, synthesis, and biological evaluation of histone deacetylase inhibitor with novel salicylamide zinc binding group

Khan hashim Ali

college of pharmacy, Keimyung University, Pakistan

Introduction: Histone deacetylases (HDACs) have emerged as important therapeutic targets for various diseases, such as cancer and neurological disorders. Although a majority of HDAC inhibitors use hydroxamic acids as zinc binding groups, hydroxamic acid zinc-binding groups suffer from poor bioavailability and nonspecific metal-binding properties, necessitating a new zinc-binding group. Salicylic acid and its derivatives, well-known for their therapeutic value, have also been reported to chelate zinc ions in a bidentate fashion. This drew our attention towards replacing hydroxamic acid with salicylamide as a zinc-binding group. Methods: In this study, for the first time, compound 5 possessing a novel salicylamide zinc-binding group was synthesized and evaluated biologically for its ability to inhibit various HDAC isoforms and induce acetylation upon alpha-tubulin and histone H3 among MDA-MB-231 cells. Results: Compound 5 exhibits selective inhibition against class I HDAC isoforms (HDAC1, 2, and 3) over class II and IV HDAC isoforms (HDAC4, 6, and 11). The exposure of MDA-MB-231 cells to compound 5 efficiently induced the acetylation of more histone H3 than □-tubulin, suggesting that compound 5 is a class I selective HDAC inhibitor. Moreover, the molecular docking study indicated that the salicylamide zinc-binding group of compound 5 coordinates the active zinc ion of class I HDAC2 in a bidentate fashion.Conclusion: Overall, salicylamide represents a novel zinc-binding group for the development of class I selective HDAC inhibitors.KeywordsHistone deacetylases, zinc-binding group, salicylamide, small molecule, drug design

Oral Presentation : **MEDI.O-7**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 10:00

Chair: Kwan-Young Jung (KRICT)

Development of in vivo genome editing nanoplatform

Se-Youl Chae, Dal-Hee Min[*]

Department of Chemistry, Seoul National University, Korea

With the development of diverse genome editing technologies, CRISPR-based genome editing was developed. The CRISPR/Cas9 system can cut or edit a specific gene with high on-target efficiency and low off-target efficiency. Furthermore, it can be used universally on any targets which contain PAM sequences. Due to its superiority, precise manipulation of DNA using the CRISPR/Cas9 system became a solution to treat genetic diseases. However, practical application to genetic diseases is difficult because Cas9 ribonucleoprotein (RNP) is vulnerable to enzymatic degradation and hard to penetrate the cell membrane. Recently, nanoparticles that can carry Cas9 RNP into cells became a solution to overcome the weaknesses in the biomedical application of Cas9 RNP. Herein, we developed porous silica nanoparticles optimized for Cas9 RNP delivery into cells, named BALL. We adjusted the nanoparticles' size, pore size, and surface modification to boost cellular uptake and endosomal escape of Cas9 RNP and found optimal conditions. Cas9 RNP delivered by BALL could successfully extinguish the 40% and 20% of GFP fluorescence in vitro and in vivo, indicating that truncation of the GFP gene could affect the phenotypic difference. Then, we applied our system to the MSTN gene, the muscle suppressor gene. We intramuscularly injected the Cas9 RNP into the tibialis anterior and cut the MSTN gene. As a result, the knockout of MSTN led to muscle growth and improved motor functions, which shows potential for treating muscular dystrophy. Taken together, we showed the possibility of practical biomedical applications using CRISPR-associated RNP.

Oral Presentation : **MEDI.O-8**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 10:10

Chair: Kwan-Young Jung (KRICT)

Discovery and Synthesis of Toll-Like Receptor 7/ 8 Dual Agonist as Vaccine Adjuvant

Ayele Abera, Sunjong Yu[1], Sandesha Nayak, Avinash G V, Young-Sik Jung[1], Soo Bong Han[1,*]

Infectious Disease Therapeutic Research Center , University of Science & Technology / Korea Research Institute of Chemical Technology, Korea

[1]*Infectious Disease Therapeutic Research Center , Korea Research Institute of Chemical Technology, Korea*

Abstract Toll-like receptors (TLR) are a family of pattern recognition receptors, which detect pathogen-associated molecular fragments. TLR7/8 are endosomal TLR that recognizes viral ssRNA, and ssRNA-derived small molecules to activate innate and adaptive immune systems whose response is expressed by inflammatory cytokines, and chemokines responses. An adjuvant is a compound added to a non-live vaccine to increase efficiency of vaccine, the magnitude and quality of the adaptive immune response. Based on structure-based drug design strategies we designed and synthesized novel TLR7/8 dual agonist lead compounds. Lead optimization and structure-activity relationship studies led to the identification of potent TLR7 agonist (AD114; EC50 = 0.05 μM), TLR8 agonist (AD108; EC50 = 0.05 μM), and TLR7/8 dual agonist (AD142; EC50 = 8.75 and 10.84 μM for TLR7 and TLR8, respectively). The in vitro and in vivo cytokine production, hERG blocking, CYP inhibition, and liver microsomal stability results demonstrated that AD110 (EC50 = 1.49 and 10.30 μM for TLR7 and TLR8, respectively) taken as TLR7/8 dual agonist for further studies. The present SAR and lead optimization results provide a road map towards the identification of a more potent, selective, and safe TLR7/8 dual agonist vaccine adjuvant.Keywords: Adjuvant, Agonist, Immune Systems , Toll-like Receptor

Oral Presentation : **MEDI.O-9**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 10:20

Chair: Kwan-Young Jung (KRICT)

Antioxidative and anti-inflammatory activity of psiguadial B and its halogenated analogues as potential neuroprotective agents

Kyungjin Jung, Jungwook Chin*

New Drug Development Center, Daegu Gyeongbuk Medical Innovation Foundation, Korea

Psiguadial B, and its fluoro-, chloro-, and bromo- derivatives were synthesized using a sodiumacetate-catalyzed single step coupling of three components: β-caryophyllene, diformylphloroglucinol,and benzaldehyde. These compounds efficiently and dose-dependently decreased H2O2-induced cell death, aquantitative marker of cell death, in primary cultures of mouse cortical neurons. Psiguadial B also decreasedneuronal death and accumulation of ROS induced by FeCl2 in cortical cultures. The in vitro effects of thesecompounds in lipopolysaccharide (LPS)-induced expression of nitric oxide (NO), and TNF-α and IL-6 by suppressingthe NF-κB pathway in immune cells demonstrated their antioxidative and anti-inflammatory activity.The present findings warrant further research on the development of psiguadial B-based neuroprotective agentsfor the treatment of neurodegenerative diseases, acute brain injuries and immunological disorders.

Oral Presentation : **MEDI.O-10**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 10:30

Chair: Kwan-Young Jung (KRICT)

Design and Synthesis of Quinazolin-4-one analogues for selective Histone Deacetylase-6 Inhibitors

Young Ho Seo[*], Sunil kumar Gupta

College of Pharmacy, Keimyung University, Korea

Quinazolinone is a well-known heterocyclic moiety that is widely used in drug discovery endeavors. We designed, synthesized, and biologically evaluated quinazolin-4-one analogues having hydroxamic acid moiety for selective HDAC6 inhibitors. HDAC enzyme assay was performed for all the molecules as a result the most potent and selective compound **5b** (IC_{50}, 17 nM, HDAC6; IC_{50}, 328 nM, HDAC1) showed better anti-proliferative effects against MCF-7/ADR cell line (GI_{50} = 2.4 µM; 72h). Furthermore, compound **5b** was able to cause the acetylation of α-tubulin at concentration as low as 0.5 µM, but not that of Histone H3 and 1 µM of compound **5b** suppressed the colony formation by 65%. Compound **5b** at a concentration of 2 µM significantly induced early and late apoptosis by 24.6 % and 15.1 %, respectively. These results were further substantiated via the induction of apoptotic signaling pathways.

Oral Presentation : **MEDI.O-11**

Oral Presentation of Young Medicinal Chemists

Room 302 THU 10:40

Chair: Kwan-Young Jung (KRICT)

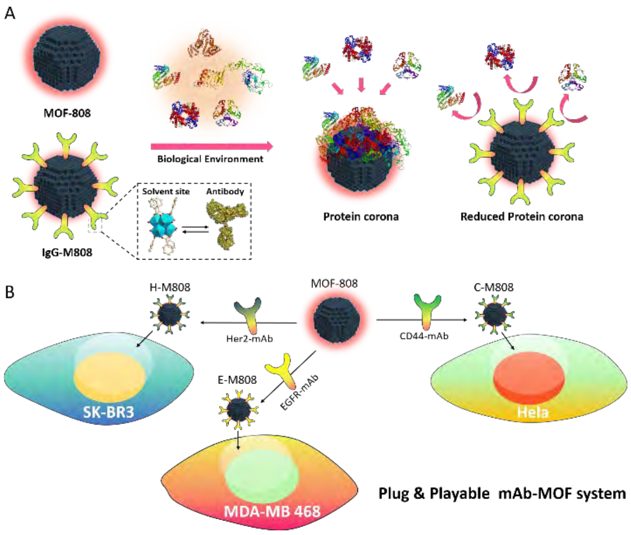
Immunoglobulin G (IgG) coated Metal-organic framework for reducing biomolecular corona

Jun Yong Oh, **Ja-Hyoung Ryu**[1,*]

Department of Chemistry , Ulsan National Institute of Science and Technology, Korea

[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Targeted delivery systems (TDS) based on metal-organic framework (MOF) has been emerged with tremendous progress and made significant attention of many scientific fields. However, translating MOF agents directly into TDS still remains a challenge due to biomolecular corona phenomenon. Once the particle is exposed to biological environment, its surface is covered with various protein by forming protein corona. Here, we show that the pre-absorption of immunoglobulin G (IgG) to the surface of MOF particle can reduce protein corona as a shield. The surface IgG are not easily exchanged nor covered by biomolecule protein and enhance the permeability of IgG-MOF complex in in-vitro and in-vivo. Based on this discovery, we introduce the plug & playable targeting systems between targetable antibodies and MOF particles. This study could provide the insight into the use of 'antibody pre-absorption' as a promising method for making a MOF based drug delivery systems.


A
MOF-808
Biological Environment
Protein corona
Reduced Protein corona
IgG-M808
Solvent site
Antibody
B
H-M808
MOF-808
C-M808
Her2-mAb
CD44-mAb
E-M808
EGFR-mAb
SK-BR3
Hela
MDA-MB 468
Plug & Playable mAb-MOF system

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Oral Presentation : **MAT.O-1**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 09:00

Chair: Chang Bum Jo (Inha University)

Highly Stable MEMS Capacitive Photodetector Based on Azobenzene-incorporated Photoresponsive Polymer

Sehun Jang, Dongjun Kim, Jiyeon Lee, Geonho Kim, Seoyoung Yoon, Jiwon Kim*

School of Integrated Technology, Yonsei University, Korea

Visible-light photodetectors have been widely used for various optoelectronic applications, such as imaging, environmental monitoring, chemical analysis, and optical communications. Conventionally, most of visible-light photodetectors have been demonstrated with p-n junction, heterojunction, or Schottky junction structures, and are based on photocurrent generation. However, current stress continuously applied to the semiconductor layer during the operation process induces degradation of the semiconductor and shortens the lifespan. Herein, we introduce a novel microbridge-structured micro-electromechanical systems (MEMS) capacitive photodetector composed of photoresponsive polymer and metal bilayer. Azobenzene-incorporated polydimethylsiloxane (AzoPDMS) was coated onto the Ni microbridge which was formed by patterning and releasing a sacrificial polyimide layer. Bilayer microbridge was deflected upon light irradiation (400-700 nm white light, 0-3 mW) due to volume expansion, which induces a change in capacitance with the fixed bottom electrode. Under 3 mW white light irradiation, capacitance changed from 10 to 13 pF, which was well-maintained even after 30 times of repeats. Moreover, we implemented an optical fiber in which the intensity of light changes upon an applied strain. This enables the developed MEMS capacitive photodetector to function as a strain sensor. Our approach is novel in that it is the first MEMS capacitive photodetector which operates via changes in morphology of photoresponsive material without constant current stress. Furthermore, we believe that the developed MEMS capacitive photodetector can be extended to various optoelectronic fields such as switches, variable capacitors, sensors, and memories.

Oral Presentation : **MAT.O-2**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 09:10

Chair: Chang Bum Jo (Inha University)

Design of Azo-integrated Covalent Organic Frameworks as Electrodes for Lithium-ion Batteries

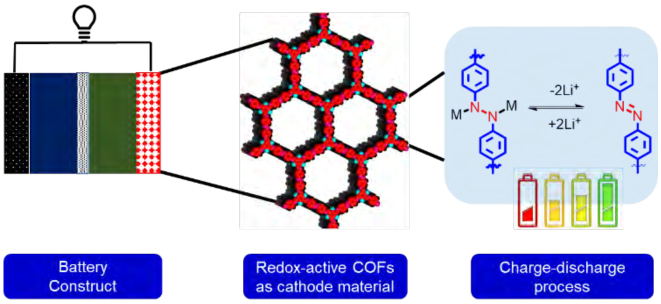
Vikram Singh, Jaewook Kim[1], Woo youn Kim[2,*], Hye Ryung Byon[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, India

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

[2]*Department of Chemistry, KAIST, Korea*

Covalent Organic Frameworks (COFs) are two-dimensional, porous, and crystalline organic structures. The well-established frameworks provide ordered mesopores, structural stability, high density, and negligible solubility, particularly attractive for battery electrodes. By integrating a redox-active azo group to COFs, we designed positive organic electrodes and applied these electrodes for nonaqueous Li-ion batteries. The azo group can undergo two electrons transfer, whereas its reversibility and stability are highly dependent on adjacent functional groups. We developed three azo-integrated COFs with three different linkages, β-ketoenamine, imine, and thiazole-fused ring. These azo-COFs had identical hexagonal $P^{6/m}$ space groups, ~3 nm of pore size, and 600~1000 m^2 g^{-1} of surface area. However, the redox chemistries of azo groups were remarkably distinct from the linkages. The β-ketoenamine and imine based azo-COFs showed irreversible azo reactions, resulting in poor capacity retention. In contrast, the fully conjugated COF containing the thiazole-fused ring rendered excellent cycling stability showing 5000 cycles at 10 C. The reversible azo reaction was also demonstrated by using operando Raman spectroscopy. This is related to the single and sharp redox wave at a formal potential of ~1.7 V vs. Li/Li^+, suggesting the one-step two electrons transfer. The solid electrolyte interphase (SEI) was formed at the initial cycles only, which could protect the COF surface and inhibit the continuous decomposition of the electrolyte solution. Electrochemical impedance spectroscopy (EIS) revealed the low charge transfer resistance (~18 Ω), which decreased further after 20 cycles (~6 Ω). The mass transport region in the EIS curve was retained, indicating the access of Li^+ to the bulk COF structure through mesopores for cycling. In the presentation, I will discuss the details of COF designs and the role of linkages enhancing the reversible and stable redox reactions in Li-ion cells.


M
N
N
M
-2Li+
+2Li+
N
N
Battery Construct
Redox-active COFs as cathode material
Charge-discharge process

Oral Presentation : **MAT.O-3**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 09:20

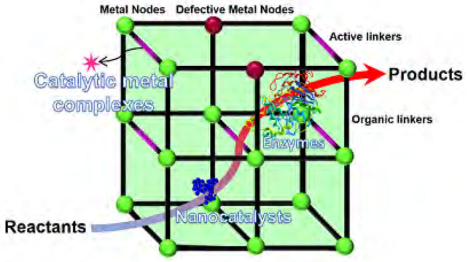
Chair: Chang Bum Jo (Inha University)

Stabilization of catalytic species within MOF-based nanoreactors: Strategies and applications

Soumen Dutta, In Su Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Rational engineering and assimilation of diverse chemo- and biocatalytic functionalities in a single nanoreactor is highly desired for effective catalytic reactions but has remained elusive. Metal-organic frameworks (MOFs), owing to the remarkable progress that has been made toward developing flexible and easy synthetic methods, diversified chemical functionalities, tunable pore structures, and low cost, have become an attractive choice as the shell material for catalytic nanoreactors.1 A porous MOF shell can be combined with an in-house nanocatalyst to deliver a selectively transformed product with maintaining the performance under recycling tests. Also, methodically engineered large pores within MOFs can allow the integration of various important large-sized catalytic species, and the functional groups of the designed linkers of MOF could stabilize them effectively. In chapter I, multimodal catalytic nanoreactors (MCNRs) based on a mesoporous MOF consisting of customizable metal nanocrystals, stably anchored enzymes, and coordinatively unsaturated cationic metal MOF nodes within a single nanoreactor space has been designed.2 The highly intimate and diverse catalytic mesoporous microenvironments and facile accessibility to the active site in the MCNR enables the cooperative and synergistic participation from different catalyst components to carry out one-pot multistep cascade reactions. Chapter II describes a unique wet-chemical anisotropic etching that creates patterned porosity on two-dimensional MOF surfaces. Then, the open pores are utilized to load molecular catalysts for an efficient energy conversion application.1. Dutta et al. Mater. Chem. Front. 2021, 5, 3986–4021.2. Dutta et al. Angew. Chem., Int. Ed. 2020, 59, 3416–3422.


Metal Nodes
Defective Metal Nodes
Active linkers
Catalytic metal complexes
Products
Organic linkers
Enzymes
Nanocatalysts
Reactants

Oral Presentation : **MAT.O-4**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 09:30

Chair: Chang Bum Jo (Inha University)

A designer approach to copper sulfide-based nanocatalysts for electrochemical nitrogen reduction: Morphology and Dopant

Haneul Jin, Hyun S. Park[1,*], Sung Jong Yoo[2,*]

Center for Hydrogen•Fuel Cell Research, Korea Institute of Science and Technology, Korea

[1]*Hydrogen Fuel Cell Research Center, Korea Institute of Science and Technology, Korea*

[2]*Fuel Cell Research Center, Korea Institute of Science and Technology, Korea*

Heterogeneous catalysis significantly depends on the surface characteristics. Therefore, developing catalysts with reaction-orienting surface energy and atomic coordinates are foremost requirements for efficient catalysis. Despite the rapid development of diverse catalysts and synthetic methods, correlating the intrinsic performances of electrocatalysts and material properties remains a challenge. Especially for multi-electron participating reactions such as electrochemical nitrogen reduction reaction (eNRR), rational design strategies for obtaining promising catalysts are very limited. Therefore, there is a pressing need to decode the catalyst properties–eNRR relations. Here we studied the relation of atomic arrangements/surface properties and eNRR performances through morphology and heteroatom doping. To test our idea, we prepared Cu1.81S nanoparticles which have two types of exposed facets of {100} and {010}. The effects of surface morphology and properties on eNRR were investigated by TEM, CV, and DFT analyses and it is discovered that the eNRR performances are highly related to the dopants and surface geometry.

Oral Presentation : **MAT.O-5**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 09:40

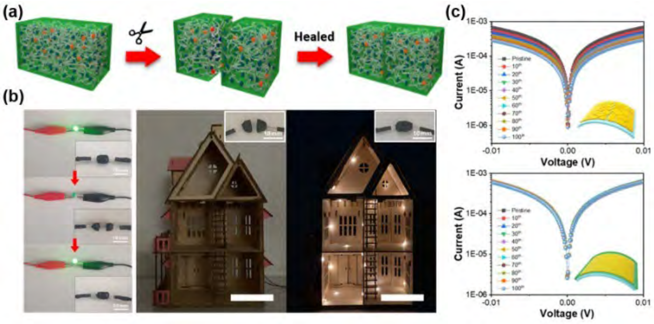
Chair: Chang Bum Jo (Inha University)

Conductive Self-Healable Rhenium Oxide-Poly(tetrahydrofuran) Composite for Resilient Flexible Electrode

Byeong-Yong Jeong, **Seok Min Yoon**[1,*]

Department of chemistry, Wonkwang University, Korea
[1]*Department of Chemistry, Wonkwang University, Korea*

The advent of flexible electronics has brought infinite varieties for their powerful penetration into many fields of smart electronics, including artificial e-skin, flexible touch sensors, health monitors, implantable devices, and so on. Metal electrodes such as gold and silver are crucial components for constructing flexible electronic circuits. However, such metal electrodes spontaneously caused cracking by a mechanical strain diminishing their original electrical conductivity. Nevertheless, surprisingly, developing methods to prevent such cracking has not been unnoticed well compared to advanced new flexible polymer conductors. Here, a novel self-healable Rhenium Oxide-poly(tetrahydrofuran) composite will be introduced, and it is used as a coating layer to prevent cracks of the metal electrodes from retaining their conductivity. The ReOX-PTHF composite exhibited high electrical conductivity of 6.4 S/cm was measured by four-point probe resistivity measurement. ReOX-PTHF composite can be easily polymerized by dissolving Re2O7 in tetrahydrofuran (THF). The Re2O7, as strong Lewis acid, can initiate ring-opening polymerization of the THF. Further, the gel rapidly healed after returning the strain back to 0.5% (for 120 s), which was almost turned back to its initial viscoelastic profile. The ReOX-PTHF composite coated Au electrodes could successfully retain their original electrical conductivity even after 100 times mechanical bending cycles. Further, the electronic circuit coupled with conductive ReOX-PTHF composite could turn on LED bulbs. The lighted LED immediately went off when the circuit was cut off, while the self-healable ability of the ReOX-PTHF composite could recover the electric power supply for turning on the bulb again.


(a)
Healed
(b)
10 mm
(c)
Current (A)
Voltage (V)
1E-03
1E-04
1E-05
1E-06
-0.01
0.00
0.01
Pristine
10th
20th
30th
40th
50th
60th
70th
80th
90th
100th

Oral Presentation : **MAT.O-6**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 09:50

Chair: Chang Bum Jo (Inha University)

25 cm2-sized Glass-like Transparent Crystalline Silicon Solar Cells with an Efficiency of 14.5%

Jeonghwan Park, Kangmin Lee, Kwanyong Seo*

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

Forming light-transmitting structures on c-Si photovoltaics to transmit visible light without wavelength dependency is a promising strategy to realize neutral-color transparent c-Si photovoltaics (c-Si TPVs). However, dry etching, which is used to form a light-transmitting structure on c-Si, inevitably causes nanoscale surface damages such as scallops and plasma-induced damage in c-Si. This aggravates carrier recombination, which decreases the power conversion efficiency (PCE) of c-Si TPVs. Here, we propose an effective chemical treatment method for removing nanoscale surface damage from c-Si microholes. A large-sized neutral-color c-Si TPV after the chemical treatment exhibited a high PCE of 14.5% at a transmittance of 20%. The chemical treatment also enabled systematic control of the hole size (167 nm/sec), and thus, the transmittance was easily tuned from 10% to 70%. Notably, the proposed chemical treatment satisfies the three development factors of 1) high PCE, 2) scaling up, and 3) easy light transmittance tuning of c-Si TPVs.

Oral Presentation : **MAT.O-7**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 10:00

Chair: Chang Bum Jo (Inha University)

Growth of Monolayer and Multilayer MoS_2 Films by Selection of Growth Mode: Two Pathways via Chemisorption and Physisorption of an Inorganic Molecular Precursor

Chaehyeon Ahn, Hyunseob Lim*

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Although various methods for growth monolayer MoS_2 using chemical vapor deposition have been attempted, homogeneous monolayer MoS_2 film with high crystallinity for short growth time is still challenging. Recent advanced synthetic methods can solve these drawbacks1,2, but the growth mechanism of MoS_2 is still unveiled clearly. Understanding the growth mechanism is very important for synthesizing high quality MoS_2, there are many attempts to understand the mechanism. Especially, some papers reported that addition of NaCl forms intermediates with low melting points facilitating the growth of MoS_2. Herein, we present another synthetic method using $MoOCl_4$, penta-coordinated inorganic complex as Mo precursor and H_2S as S precursor. The thickness of grown MoS_2 sample can be controlled by precursors pressure, i) physisorption ii) chemisorption. At the low growth pressure, we can synthesis thin film of MoS_2 at even 50 min growth time because chemisorption between substrate and $MoOCl_4$ occurs and physisorption between MoS_2 and $MoOCl_4$ rarely occurs. At the high growth pressure, in contrast, both chemisorption and physisorption of $MoOCl_4$ on a quartz substrate can occur, which results in thicker MoS_2 film grown with higher growth rate, because the partial pressure of $MoOCl_4$ is high enough. Furthermore, the density functional theory (DFT) has been carried out to support the mechanism we suggest. Our growth method also facilitates the growth of MoS_2 film having negligible carbon contamination, since all precursors used in the reaction do not consist of any carbon element. We believe that our demonstrations do not only provide the fundamental insight to understand the precise growth mechanisms of MoS_2, but also enables the thickness-controllable growth of high-quality monolayer MoS_2 film.

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2. J. Zhou, J. Lin, X. Huang, Y. Zhou, Y. Chen, J. Xia, H. Wang, Y. Xie, H. Yu, J. Lei, Nature 2018, 556, 355.

Oral Presentation : **MAT.O-8**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 10:10

Chair: Chang Bum Jo (Inha University)

Highly luminescent and catalytically active suprastructures of magic-sized semiconductor nanoclusters

Megalamane siddaramappa Bootharaju, Taeghwan Hyeon[1,*]

Center for Nanoparticle Research, Seoul National University, Korea
[1]*Division of Chemical & Biological Engineering, Seoul National University, Korea*

Metal chalcogenide magic-sized nanoclusters (MSCs) have shown intriguing photophysical and chemical properties, yet ambient instability has hampered their extensive applications. Here we explored the periodic assembly of these nanoscale building blocks through organic linkers to overcome such limitations and further boost their properties. We designed a diamine-based heat-up self-assembly process to assemble Mn2+:(CdSe)13 and Mn2+:(ZnSe)13 MSCs into three- and two-dimensional suprastructures (SSs), respectively, obtaining enhanced stability and solid-state photoluminescence quantum yields (from

Oral Presentation : **MAT.O-9**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 10:20

Chair: Chang Bum Jo (Inha University)

Improvement of the Energy-Functionality of Nanostructured Materials via the Hybridization with Multilayered Conductive Nanosheet

Namhee Kwon, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

The hybridization with conductive nanospecies has evoked great deal of research activities because of its usefulness in improving diverse energy-functionalities of nanostructured materials. In this study, a novel synthetic route for exploring high-performance energy-functional materials is developed by employing multilayer conductive 2D hybrid nanosheet of graphene/metal oxide/graphene as a new type of conductive hybridization matrix. The self-assembly between anionic MoS_2/MnO_2 nanosheets (NSs) with polycation-anchored cationic reduced graphene oxide (prGO)/RuO_2/prGO NSs yields the 2D superlattice nanohybrids. Using robust prGO/RuO_2/prGO nanosheet as a hybridization matrix is quite effective in improving the structural ordering of hybridized species with the depressed crystal defect formation and enhancing the porosity of the nanohybrids. As a result, the multilayer conductive nanosheet-based hybrids deliver much superior electrocatalyst and supercapacitor electrode performance over the single-layered rGO or RuO_2 nanosheet-based hybrids. The superior advantages of multilayer conductive nanosheets originate from the enhancement of charge/mass transports caused by the flattening of hybridized 2D crystallites and the increase of porosity. The universal usefulness of multilayer nanosheet is cross-confirmed by profound effect of stacking pattern on the electrocatalyst functionality of layer-by-layer-deposited MoS_2/rGO/RuO_2 films.

Oral Presentation : **MAT.O-10**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 10:30

Chair: Chang Bum Jo (Inha University)

Oxidation-resistance of copper nanoparticles with excess electrons

Kyungwha Chung

Institute of Quantum Biophysics, Sungkyunkwan University, Korea

Copper nanoparticles (NPs) have received extensive interest owing to the technical merits compared to bulk counterparts. Although the natural oxidation of Cu NPs has been avoided by passivating the surfaces with additional moieties, non-oxidized bare Cu NPs in air are still challenging. Here, we report that bare Cu NPs with surface excess electrons retain non-oxidized state over several months in ambient air. The Cu NPs grown on the electride support with excellent electron transfer ability are encapsulated by the surface-accumulated excess electrons, exhibiting decreased work function (~3.2 eV). Atomic-scale structural and chemical analyses confirm the absence of Cu oxide at the outermost surface of air-exposed bare Cu NPs. Calculated energetics clarify that the surface-accumulated excess electrons suppress the oxygen adsorption and consequently prohibit the infiltration of oxygen into Cu lattice, provoking the endothermic reaction for oxidation process. Our results will further stimulate the practical utility of metal NPs in versatile applications.

Oral Presentation : **MAT.O-11**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 10:40

Chair: Chang Bum Jo (Inha University)

Supercooled Liquid Intermediate State: Origin of Lattice disorder in Rubrene Crystals Revealed by in Situ Physical Vapor Transport Process

Youngkwan Yoon, Hee Cheul Choi[1,*]

Chemistry, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

The physical vapor transport (PVT) process is one of the most popular techniques for the formation of organic thin films or functional organic crystals. Especially, rubrene crystals obtained by PVT process are one of the most popular organic crystals by electronics materials scientists for their highest charge carrier mobility. However, the formation of lattice disorder during crystallization deteriorates mobility, and controlling the lattice disorder remains a challenge due to the lack of understanding of crystal growth in PVT process. Here, we present that the crystallization by PVT undergoes a supercooled liquid (SCL) intermediate state depending on the crystal growth condition, which affects the formation of lattice disorder in rubrene crystals. The SCL intermediate state is observed by in situ & real-time optical images, Raman, and photoluminescence (PL) analyses, providing new insights into the crystallization mechanism of the PVT method. Furthermore, we found the relation between the SCL intermediate state and lattice disorder by Raman and PL analysis, and improved the charge carrier mobility by about 5 times through the control of SCL intermediate states. Our studies will provide the key understanding of organic crystal growth by PVT, through which great opportunities for various practical applications by controlling the lattice disorder will be available.

Oral Presentation : **MAT.O-12**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 10:50

Chair: Chang Bum Jo (Inha University)

Automated Synthesis of Coke-Resistant Cs-Promoted Ni/Al_2O_3 Nanocatalyst for Dry Reforming of Methane

Kyung Hee Oh, Chang Seop Hong[1], Ji Chan Park[*]

Clean Fuel Laboratory, Korea Institute of Energy Research, Korea
[1]*Department of Chemistry, Korea University, Korea*

Dry reforming of methane (DRM) is an eco-friendly process to produce syngas (CO, H_2) from greenhouse gases (CH_4, CO_2). In the catalytic reaction, various Ni-supported catalysts have been employed, but improving stability against coke deposition and increasing productivity in the catalysts are still major issues. Herein, we newly report the Cs-promoted Ni/Al_2O_3 nanocatalyst with a very high Ni load of 30 wt% and uniform dispersion with very small particle sizes (ca. 5 nm), prepared via a facile melt-infiltration route in the all-in-one automated apparatus designed for the synthesis of solid catalysts. As the results of the DRM reaction test at 800 °C, the obtained nanocatalyst almost reached the equilibrium conversion even at extremely high space velocity conditions (~72 $NL\cdot g_{cat}^{-1}\cdot h^{-1}$) as well as much enhanced coke-resistance, compared to those of conventional Ni/Al_2O_3 catalyst and commercial Ni catalyst.

Oral Presentation : **MAT.O-13**

Oral Presentation for Young Material Chemists

Tamna Hall C THU 11:00

Chair: Chang Bum Jo (Inha University)

Confinement of gold nanoparticles in commercial zeolites by post-functionalization method

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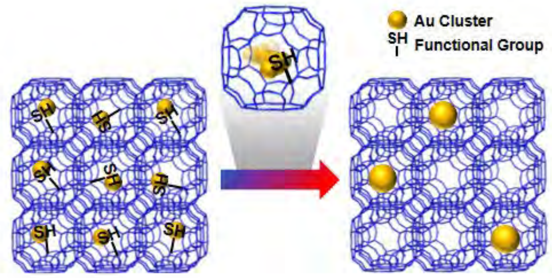
Gold has attained more attraction after it is found active in numerous chemical reactions. The limitation is to obtain gold nanoparticles less than 10nm in size. Also, it suffers from active metal sintering. In this study, post-functionalization was followed to prepare gold nanoparticles encapsulated in zeolite micropores, that has resistance towards sintering. The prepared sample were characterized using X-ray diffraction, NMR, TGA and sorption. The STEM results ensured that gold particles are in well-dispersed form having an average particle size of 1-2 nm after thermal treatment. Following this route, the catalysts obtain were having gold nanoparticles inside zeolite micropores. This was further confirmed by small and bulky alcohol oxidation. Compared to conventional incipient wetness method, these catalysts have about twenty times enhanced catalytic activity towards CO oxidation and acetylene hydrogenation.



Oral Presentation : **ELEC.O-1**
Oral Presentation of Young Scholars in Electrochemistry
Room 402 THU 09:00
Chair: Hye Ryung Byon (KAIST)

Engineering the electronic structure of single atom catalysts for electrochemical CO2 reduction

Rami Reddy Boppella, Tae Kyu Kim[1,*]

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Atomically dispersed and nitrogen coordinated single metal sties (M–N–C) embedded in carbon support have exhibited exceptional catalytic activity and selectivity for the electrochemical CO2 reduction reaction (CO2RR) to CO. However, due to constrained synthesis approaches and a lack of ability to precisely characterize the specific local environment, establishing a definitive link between structure and performance is extremely difficult. A soft-template aided technique is developed for the first time to synthesize a pyrrolic N4–Ni sites coupled with varying N-type defects to synergistically enhance the CO2RR performance. The soft template was crucial in regulating the electronic structure of Ni-N–C catalysts. The monotonous effects of N-type dopant on the CO2RR were comprehensively elucidated. Results of controlled experiments exposed that metal free defect sites are primary active sites for the CO2RR rather than the single-atom Ni–N4 sites. Theoretical calculations revealed that carbon atoms next to pyrrolic N have a lower energy barrier for the reaction intermediates, and the pyrrolic N of Ni–N4 sites, rather than Ni sites, serve as preferential CO desorption sites. The pyrrolic N in Ni–N4 and N-doped carbon regulate the electronic structure of the catalyst, resulting in lower CO2 adsorption energy and higher intrinsic catalytic activity.

Oral Presentation : **ELEC.O-2**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 09:10

Chair: Hye Ryung Byon (KAIST)

Electrocatalytic CO2 Reduction to C2 Products: Tuning of Product Selectivity by Copper Doping over Ag-Complex-Carbon Hybrid

Balamurugan Mani, Nam Ki Tae[1,*]

Department of Materials Science and Engineering, Seoul National University, Korea

[1]*Division of Material Engineering, Seoul National University, Korea*

Selective electrochemical conversion of CO2 to hydrocarbons in aqueous media is really challenging because of the multiple proton-coupled electron transfer processes and the dominant hydrogen evolution as a side reaction. In particular, selective production of C2-Cn products from CO2 is really beneficial but disfavoured by many factors. To date, copper is the ideal metal that favors the C-C coupling and hydrocarbons production from CO2 and appreciable efforts have been made previously to enhance the C2 selectivity and current density. In this study, the silver molecular complex has been immobilized on graphitized mesoporous carbon (GMC) and acts as efficient catalysts for highly selective CO production. Interestingly, copper ion doping over the Ag-complex-carbon hybrid (Ag-NTB-GMC), the selectivity is completely shifted and the C2 selectivity is enhanced up to 75% in KCl solution. The observation of C2 product clearly reveal that the cooperative effect of Cu-Ag for the enhanced CO2 reduction process. Further, it was found that the Cu-Ag alloyed nanoparticle, as well as very small size nano-cluster of Ag and Cu, decorated over the GMC acts as the active site during the electrocatalytic CO2 reduction reactions.

Oral Presentation : **ELEC.O-3**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 09:20

Chair: Hye Ryung Byon (KAIST)

Permeabilization-free β-Galactosidase-Induction-Based Electrochemical Detection of *Escherichia coli*

Jungwook Kwon, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Escherichia coli (*E. coli*) is recognized as an indicator of fecal bacterial contamination, and the induction of intracellular β-galactosidase (Gal) is commonly used for sensitive and selective *E. coli* detection. However, this method requires a simple procedure to ensure that the Gal substrate and product are highly permeable through the *E. coli* membrane, making it unsuitable for simple point-of-care detection. Here, we report a sensitive electrochemical method for *E. coli* detection that does not require a permeabilization process. Intracellular Gal expression is increased via induction by isopropyl-β-D-thiogalactopyranoside (IPTG). 4-Methoxyphenyl-β-D-galactopyranoside (MPGP) and 4-methoxyphenol (MP) are used as the highly cell-permeable Gal substrate and product, respectively. Externally-added tyrosinase (Tyr) converts MP into electrochemically active 4-methoxycatechol, which is then electrochemically oxidized via electrochemical-chemical redox cycling involving an electrode, 4-methoxycatechol, and tris(2-carboxyethyl)phosphine. The presence of MPGP during the induction of intracellular Gal led to amplified MP production. The results of four different detection methods using three Gal substrates (MPGP, phenyl-β-D-galactopyranoside, and 4-aminophenyl-β-D-galactopyranoside) were compared. The detection limit for both drinking water and tap water spiked with *E. coli*, obtained following a 2-h-long IPTG treatment and 5-min-long Tyr reaction, was ~2×10^3 colony-forming units (CFU)/mL, indicating that this method can be applied to monitoring *E. coli* contamination in water samples. Importantly, the present method does not require the electrode modification, affinity binding, washing, and filtration steps.

Oral Presentation : **ELEC.O-4**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 09:30

Chair: Hye Ryung Byon (KAIST)

Improved stability of LiCoO$_2$ cathode with kosmotropic anions in aqueous lithium-ion batteries

Hyunjeong Oh, Hye Ryung Byon[1,*]

Korea Advanced Institute of Science and Technology, Korea

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Aqueous rechargeable lithium-ion batteries have been recently highlighted for the low-cost and safe energy storage systems. However, layered-structure of LiCoO$_2$ (LCO) as the positive electrode has suffered from low stability in aqueous electrolyte solution, because protons are easily intercalated to the Li vacancy and change both bulk and surface structure. Here, we studied the interfacial reaction between LCO electrodes and aqueous electrolyte solution containing various lithium salts (Li$_2$SO$_4$, LiNO$_3$, LiClO$_4$, and LiTFSI) with 0.5~1 mol/kg concentration. We show that structural deformation of the LCO is associated with anions of electrolytes, determining galvanostatic cycling performances. In particular, the kosmotropic and chaotropic characteristics of anions, following Hofmeister series, significantly affect the interfacial reaction. The H+ insertion is pronouncedly reduced with the kosmotropic anions (SO$_4^{2-}$) and attribute to the improved cyclability, from the rigid water-solvation shell and the formation of the ion pairs between Li$^+$ and SO$_4^{2-}$ at the electrode. It suggests the controllable water and proton motion by anions at the electrode surface and attribute to the improved cycle performance.

Oral Presentation : **ELEC.O-5**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 09:40

Chair: Hye Ryung Byon (KAIST)

Identification of Active Sites for CO_2 Electroreduction Using Atomically Precise Gold Nanoclusters

Hoeun Seong, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Precise identification of active sites for specific reactions is critical for comprehending mechanisms of catalytic reaction and designing highly efficient and selective catalysts. Here, I present the identification of active sites for electrochemical CO_2 reduction reaction (CO_2RR) using atomically well-defined gold nanoclusters (Au NCs): $Au_{25}(SR)_{18}$, $Au_{38}(SR)_{24}$, and $Au_{144}(SR)_{60}$, where SR is a thiolate ligand. The Au NCs showed extraordinary CO_2RR activity, which increased with increasing their size, with exhibiting high selectivity for CO production (>90%) at entire studied regions. Combining electrochemical and X-ray photoelectron spectroscopy analyses, it was revealed that the Au NCs were electrochemically activated by losing one thiolate ligand (i.e., dethiolation) from each staple motif during electrocatalysis. Furthermore, density functional theory calculations predicted that staple Au sites of the Au NCs are the active sites for CO_2RR. It was also expected that the active sites become more negatively charged and the d-states of them upshift via dethiolation, and thereby accelerate the CO_2RR. The structure–activity relations of the Au NCs clearly indicated that the dethiolated Au sites were the active sites for CO_2RR, and the activity was determined by the number of active sites on the NCs.

Oral Presentation : **ELEC.O-6**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 09:50

Chair: Hye Ryung Byon (KAIST)

In-Depth Micro-Kinetic Study of Concentration Effects on the Electrochemical Reduction of CO_2 (CO_2RR) on Copper Catalyst.

Kamal Asghar

Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

Almost all the technologies we rely on in our lives are powered by fossil fuels. The continuous and extensive use of fossil fuels across the world releases billions of tons of CO_2 into the atmosphere which is connected to potential global warming. Therefore, the electrochemical reduction of CO_2 into valuable chemicals is one of the promising approaches for the storage and conversion of sustainable energy. Herein, we present a refinement of a previously developed microkinetic modeling approach [Nature Comm. 2019, 10, 32.] for CO_2 reduction reaction (CO_2RR) on the surface of the Cu electrode towards mono carbon and multicarbon products. Using the microkinetic modeling package CatMAP, we evaluated the turnover frequency of all products as a function of CO_2 partial pressure and pH. We will show the direct relationship among *CO-coverage, current density, reaction order, and rate-determining steps of all products. Further, we bring here another issue that's what will be the effect of local CO partial pressure during the CO_2RR? Because the produced CO(g), during the CO_2RR, is re-absorbed on the catalyst surface giving the pathway for the CORR. Hence, by fixing different CO_2 partial pressure, we evaluated the activity of the catalyst as a function of local CO partial pressure and pH. Therefore, this work will deliver some scientific conclusions that will help to understand the role of local CO partial pressure in CO_2RR mechanistically.

Oral Presentation : **ELEC.O-7**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 10:00

Chair: Hye Ryung Byon (KAIST)

Characteristics of Grain boundary in bimetallic Pt-Co nanowires for oxygen reduction reaction (ORR) performance

Mrinal kanti Kabiraz, Chang Hyuck Choi[1], Sang Woo Han[2], Sang-Il Choi[3,*]

Kyungpook National University, Korea
[1]*Gwangju Institute of Science and Technology, Korea*
[2]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*
[3]*Department of Chemistry, Kyungpook National University, Korea*

Grain boundaries (GBs) as defects are considered highly active sites for many electrochemical reactions. Previously, the presence of the GBs considered beneficial for the cathodic oxygen reduction reaction (ORR) in the fuel cells owing to its optimal coordination environment. For the first time, our study indicates that GBs in bimetallic Pt-Co alloys are not beneficial in terms of the leaching of non-noble metals during the electrochemical process. GBs-containing Pt-Co nanowires (Pt-Co GB-NWs) and GBs-free single-crystalline Pt-Co NWs (Pt-Co SC-NWs) are synthesized to investigate such adverse behavior. Except for GBs, two types of NWs contained similar Pt/Co ratios, similar ultrathin diameters, and Pt-skin-like surface structures. In-operando inductively coupled plasma-mass spectroscopy (ICP-MS) reveals that, during the activation process, more Co atoms were leached from Pt-Co GB-NWs than Pt-Co SC-NWs. After activation, the Pt-Co SC-NWs exhibited superior ORR mass activity of 2.54 A mg-1Pt which is 1.9 times higher than Pt-Co GB-NWs. Therefore, the presence of GBs promoted Co leaching from Pt-Co NWs/C, resulting in stronger *OH binding and reduced ORR activity.

Oral Presentation : **ELEC.O-8**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 10:10

Chair: Hye Ryung Byon (KAIST)

Electrochemical Detection of an Individual Blood Cell Based on an Ultramicroelectrode

Jungeun Lee, Seungwoo Hong[1], Byung-Kwon Kim[2,*]

Department of Chemistry, Department of Chemistry and Nanoscience, Korea
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[2]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*

Blood cells present in blood vessels are involved in various reactions directly related to survival problems, such as oxygen transport, immune response, and homeostasis in the human body. In particular, diseases caused by more than the average size or number of various blood cells themselves have a direct effect on survival by inhibiting homeostasis. Although there is a method that allows experienced medical staff in hospitals to report various blood cell levels based on the complete blood count (CBC), it is also necessary to develop a new point-of-care biosensor that can easily and quickly detect an approximate blood count. Therefore, this research introduces an electrochemical detection method of a blood cell using ultramicroelectrode that can be applied to biosensors.References 1. K. Kikkeri. et al. (2022) ‘A sample-to-answer electrochemical biosensor system for biomarker detection’, Lab on a Chip, 22(1), pp. 100-107.2. J. Lee. et al. (2019) ‘Stochastic Electrochemical Cytometry of Human Platelets via a Particle Collision Approach’, ACS Sensors, 4(12), pp. 3248-3256.3. T.L.T, Ho. et al. (2018) ‘Determining mean corpuscular volume and red blood cell count using electrochemical collision events’, Biosensors and Bioelectronics. 110, pp. 155-159.4. X. Wang, et al. (2017) ‘White blood cell counting on smartphone paper electrochemical sensor’, Biosensors and Bioelectronics. 90, pp. 549-557.

Oral Presentation : **ELEC.O-9**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 10:20

Chair: Hye Ryung Byon (KAIST)

Selective Olefin Epoxidation by Co-TAML electrocatalysts

Suyeon Kim, Wonwoo Nam[1,*], Sun Hee Kim[2,*], Kyoungsuk Jin[3,*]

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In the modern chemical industry, epoxides have been regarded as pivotal ingredients for chemical synthesis. In general, the reactive three-membered heterocyclic ring in epoxides can be opened by nucleophilic groups, thus easily introducing diverse functionality. Currently, thermochemical routes are employed to epoxide target olefins under elevated temperature and high pressure. Given that the whole country aims to build a carbon-neutral society, it would be essential to exploit sustainable methodologies to replace the current route.Herein, we report electrocatalytic epoxidation via the generation of Co-oxo intermediate in Co-TAML(tetraamido macrocyclic ligand) molecular catalysts. Without additional oxidants, it can epoxidize olefin substrates using water as an oxygen atom source under ambient conditions. Selectivity control of olefin oxidation is particularly important, as it can generate various oxidized products, such as corresponding ketone, alcohol, and epoxide. We confirmed that Co-TAML catalyst is able to selectively produce epoxide products using cyclohexene as a model substrate. Interestingly, we also verified that the reaction pathway between C-H activation and olefin double-bond activation could be tuned depending on the solvent/electrolytes composition. Through the condition optimization process, the target epoxide was obtained at about 20-30% Faradaic efficiency, by Co-TAML catalysts. Furthermore, to elucidate the reaction mechanism, a series of electrokinetic studies were conducted. We then tried to characterize the high valent Co(IV)-TAML oxo intermediates with spectroelectrochemical studies including Electron paramagnetic resonance (EPR) and UV-Vis spectroscopy.

Oral Presentation : **ELEC.O-10**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 10:30

Chair: Hye Ryung Byon (KAIST)

Synthesis of Core-Shell type Prussian Blue Analogues and application of a cathode material for a water-based rechargeable battery

Seohyun Park, Ji-Hoon Lee*

Head of Department of Hydrogen Energy Materials, Nano Surface Materials Division, korea Institute of Materials Science, Korea

Recently, the demand for eco-friendly energy is rapidly increasing. Accordingly, the development of a large-scale energy storage system is essential. In particular, lithium-ion batteries are attracting attention due to their high energy density and charging/discharging efficiency. However, as prices and safety problems are constantly increasing, research on aqueous secondary batteries is in the spotlight. On the other hand, Prussian Blue Analogue(PBA)-based metal-organic structures have several advantages, which has been recognized as being suitable for use as a next-generation electrode material. But there are some issues regarding of specific capacity. Therefore, in this study, V/Fe PBA, which exhibits high discharge capacity, was selected as an electrode material for cathode. At the same time, in order to prevent elution of transition metal ions in the V/Fe, Cu/Fe PBA with high stability was additionally selected and synthesized as a shell material. A cathode material having a core-shell structure was synthesized by performing a two-step co-precipitation method in succession. Accordingly, it was confirmed that there was no decrease in the initial specific capacity due to an increase in the shell thickness up to 10 mM. Consequently, it was confirmed that the synthesized V/Fe@Cu/Fe PBA improved the stability of the cathode material cycling by sufficiently protecting the core layer by forming the shell material Cu/Fe PBA on the surface. According to the results of this study, the core-shell type V/Fe@Cu/Fe PBA effectively prevents the elution of transition metals for activation and minimizes the initial specific capacity reduction to have high cycling stability. It can be applied as an electrode material for a secondary battery potentially.

Oral Presentation : **ELEC.O-11**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 10:40

Chair: Hye Ryung Byon (KAIST)

Delocalization of charges at the heterojunction of $NiCo_2S_4@SnS_2$ hybrid for improved electrochemical kinetics and enhanced supercapacitor performance

Anil kumar reddy Police

Department of Civil and Environmental Engineering, Konkuk University, Korea

Supercapacitors are considered potential energy storage devices due to their superior power density, extended cyclic stability and greater safety. But the limited charge storage capacity of the supercapacitors resulted in the lower energy densities as compared to the batteries. In this view, pseudocapacitors can be an alternative to supercapacitors because of their larger specific capacitance and greater energy densities originating from the rapid faradic redox reactions. Hence, pseudocapacitor electrode materials are explored widely to achieve the requirements of the commercial energy storage devices. Transition metal-based sulfides have high conductivity and theoretical capacitance suitable for pseudocapacitors; however, the sluggish reaction kinetics and poor cyclic stability are limited for the practical applications. Heterostructured materials with multiple metal sulfides improve the performance by offering enhanced redox-active sites and surface reaction kinetics facilitated by additional ion and electron pathways. Herein, we prepared SnS2 supported NiCo2S4 heterostructured material (NiCo2S4@SnS2) which showed 140% capacity enhancement with a capacity retention of 76.87%, and excellent coulombic efficiency of 99.77%. Computational studies revealed the formation of Co-S covalent bonds due to the interaction of Co (NiCo2S4) and S (SnS2) atoms. Bader charge analysis explained the enhanced charge density on the Co atoms that generated additional redox active sites in the NiCo2S4@SnS2 heterostructure and ultimately enhanced the electrochemical performance. An all-solid-state asymmetric supercapacitor device (NiCo2S4@SnS2//hrGO) was fabricated, that delivered high energy and power densities with an outstanding 93.8% cyclic stability for 10000 charge/discharge cycles.

Oral Presentation : **ELEC.O-12**

Oral Presentation of Young Scholars in Electrochemistry

Room 402 THU 10:50

Chair: Hye Ryung Byon (KAIST)

Isoindigo-based organic small-molecule cathodes for long cycle life and high-rate secondary batteries

Jong-Jin Park, Ji Eon Kwon*

Functional Composite Materials Research Center, Korea Institute of Science and Technology, Korea

Redox-active organic molecules (ROMs) are promising electrode materials for next-generation rechargeable batteries owing to their beneficial advantages of environmental friendliness, natural abundance, low cost, and possible high theoretical capacity. However, they suffer from a serious dissolution problem in organic electrolytes and low electrical conductivity, limiting their practical application. In particular, despite many advantages such as easy synthesis, potential low cost, and convenient processing, small-molecule electrode materials have typically showed far inferior stability and rate performance than polymeric materials.Herein, two isoindigo-based small molecules, isoindigo (Me-IIG) and thienoisoindigo (Me-TIIG), were synthesized and evaluated as a cathode material in lithium-organic batteries. In a Li coin cell, Me-IIG and Me-TIIG electrode exhibited specific capacity of 156 and 168 mAh g-1 at 1C, corresponding to 84% and 95% of capacity utilization, respectively. The Me-TIIG with better molecular planarity than the Me-IIG showed much lower solubility in organic electrolytes with the aid of strong intra- and intermolecular interactions. As a result, the Me-TIIG electrode presented remarkably improved cycling stability, retaining 80% (135 mAh g-1) of the initial capacity after 500 cycles at 1C rate. Moreover, Me-TIIG exhibited lower reorganization energy than Me-IIG, which can facilitate a kinetically faster electrochemical pathway, leading to superior rate capability. It should be noted that the Me-TIIG electrode showed excellent rate performance achieving 40% capacity retention (70 mAh g-1) at a high rate of 50C.

Oral Presentation : **EDU.O-1**

New Trends in Chemistry Education

Room 301 THU 09:00

Chair: Hyunjung Kim (Kongju National University)

A Case Study on the Difficulties of Experiments in the Course of Chemistry Research Project Experienced by Graduates of Science-Gifted Education Institute

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This study examines the difficulties of experiments in the course of chemistry research project experienced by two graduates of science-gifted education institute. The difficulties students experienced could be viewed from three aspects. First, there is an environmental aspect in that it is difficult to find a laboratory with equipment suitable for the research topic. Second, there is a functional aspect in that it is difficult to acquire the tacit knowledge required to use the equipment skillfully and to meticulously prepare a sample even if there are equipment that can be used for the experiment. Finally, in the emotional aspect, there is anxiety about high uncertainty due to the academic nature of chemistry that conducts and interprets experiments from the perspective of microscopic particles. Based on these analysis results, this study drew implications in the context of science-gifted education, chemistry education, and experimental education.

Oral Presentation : **EDU.O-2**

New Trends in Chemistry Education

Room 301 THU 09:20

Chair: Hyunjung Kim (Kongju National University)

Instructional Design with ‘Little Prince’ for Convergence Education, and It’s Implementation

Ju Ran Shin

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Fairy tales and literature provide readers with impressions, lessons, pleasures, and empathy. Futhermore, they are useful tools to make students understand the background, thoughts, scientific knowledge, ethics, and occupations of different times and cultures. Therefore, using fairy tales and literary works in class can be a great case for convergence education making it possible for students to interpret the situation from various perspectives and ultimately be involved in an integrated thinking process. For example, the educational value of using fairy tales and literary works as instructional materials can be listed as follows: motivation, and continuation of learning, expansion of imagination and creativity, developing integrated thinking and aesthetic sense, etc. Moreover, the classes using fairy tales and literary works are developed and provided as an innovative teaching method. In this study, thus, based on Saint-Exupery's Little Prince, an integrated instructional design will be developed and its educational applicabillity will be searched. The story-based inegrated instructional design consists of six stages, and the body of this paper follows its composition. Firstly, to identify and classify content elements in the story. Secondly, to link the content elements with subjects. Thirdly, to select and confirm achievement standards for each subject. Fourthly, to organize topics and set learning objectives. Fiftly, to design programs. Finally, to evaluate and reflect on the programs, which includes discussing things to consider and probable difficulties in developing and implementing this integrated instructioal design.

Oral Presentation : **EDU.O-3**

New Trends in Chemistry Education

Room 301 THU 09:40

Chair: Hyunjung Kim (Kongju National University)

Science Instructional Design of Metaverse Education Platform

HyunJu Park

Faculty of Chemistry Education, Chosun University, Korea

As interest in remote education due to the COVID-19 pandemic, attempts are being made to connect and utilize the platform Metaverse, which is recently used in all fields such as society, economy, industry, and culture, in education. Metaverse is a compound word of ‘meta’ meaning ‘virtual’ and ‘transcendence’ and ‘universe’ meaning the universe. , refers to a three-dimensional virtual world where industrial and cultural activities take place. There are methods to use metaverse platforms such as 'zepeto', 'ifland', and 'gather town' for education, and a method to design a new metaverse education platform. This study examines the process, procedure, and strategy of designing a new metaverse science education platform, and intends to provide implications and basic data for the use and development of metaverse in science education. This study also included some discussions on the educational effectiveness and value of metaverse.

Oral Presentation : **EDU.O-4**

New Trends in Chemistry Education

Room 301 THU 10:15

Chair: Hyunjung Kim (Kongju National University)

Meaning of organic synthesis activity in organic chemistry class at Korea Science Academy

Jinho Oh

Chemistry & Biology, Korea Science Academy of KAIST, Korea

Organic compounds are important materials not only in modern chemistry but also in our modern life. Organic compounds are carbon compounds. If someone ask you what did you learn in organic chemistry subjects in your college life? I think that you may say that you forget what you learned. Maybe it is true that we cannot remember any organic chemistry knowledge. Even we look for aspirin or tylenol whenever we have headache, nobody want to know the structure of aspirin. Maybe it is impossible to know the structure of all organic materials and the structures of some organic compounds are so complicate. New organic compounds are synthesized or discovered every day and are reported in newspaper or journal. Organic chemistry is essential course for chemistry or relative majors in the university and many students are required to memory organic chemistry knowledge. How many students do want to know the structure of organic compounds after the class? At Korea Science Academy, I meet students who like organic chemistry and them who have difficulties. I want that students have fun when students learn organic chemistry or chemistry. Organic chemistry text book includes hydrocarbon compounds such as alkane, alkene, alkyne, aromatic compounds and alcohols and ether compounds containing carbon-oxygen sing bond, amine compounds containing carbon-nitrogen sing bond, and aldehyde, ketone, and carboxylic acid and their derivatives having a carbonyl group. Students can learn Organic chemistry based on the reaction mechanism according to each functional group.In this presentation, I will introduce an organic synthesis project activity in the fundamental organic chemistry subject at the Korea Science Academy. The organic synthesis project activity may let students apply the knowledge learned in the course. I hope that these activities will allow students to more easily overcome the barriers of organic chemistry when they enter college.

Oral Presentation : **EDU.O-5**

New Trends in Chemistry Education

Room 301 THU 10:35

Chair: Hyunjung Kim (Kongju National University)

Elementary school students' understanding of matter and its examples

Heejun Lim, Sang-Ihn Yeo[1,*]

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[1]*General Science Education, Gyeongin National University of Education, Korea*

Matter is a basic concept that students should understand during their science classes. However, many difficulties are associated with understanding the concepts of matter due to its abstraction. In this study, the elementary school students' understanding of the concept of matter and the examples of matter and non-matter are investigated and analyzed by grade. The subjects of this study were 418 students from third grade to sixth grade. The survey was conducted using a free-response questionnaire comprising three questions. The results are as follows. First, the elementary school students’ conceptions of matter were “materials that make up objects,” “what can be seen and touched,” and “solid, liquid, and gas.” As the grade increased, the explanations for a material decreased and the explanations for the state of matter increased. Furthermore, only few students explained matter in terms of mass and volume. Second, solids were the most common examples of matter presented by the students, and liquids and gases were included in the upper grades. However, there were many cases in the upper grades where students were unable to distinguish between objects and matter. Third, non-matter was properly presented by the 6th graders as compared to the other graders, and in many cases, objects, liquids, and gases were mentioned as non-matter. Fourth, it was found that the students’ conceptions of matter influenced the examples of matter and non-matter that they presented.

Poster Presentation : **POLY.P-1**

Polymer Chemistry

Event Hall FRI 11:00~13:00

High-visibility 1D photonic crystal sensors using novel inorganic-copolymer hybrid materials: Facile colorimetric differentiation of benzene, toluene, and xylene.

Tae Gyu Hwang, Minju Jeong, Min Jeong Choi, Jong-Mok Park*

Research Center for Advanced Specialty Chemicals, Korea Research Institute of Chemical Technology, Korea

Optical properties of one-dimensional photonic crystals (1D PCs) can easily be changed according to the refractive index difference between high-and low-refractive index materials as well as their thickness changes. Based on this interesting properties, 1D PCs are being developed as a optical sensors for naked-eye detection, which requires high visibility. Herein, we propose a facile method for the fabrication of highly reflective 1D PC sensors, which exhibit large refractive index difference when immersed in liquid analyte. A photo-crosslinked titania-copolymer hybrid based novel high-refractive index material and photo-crosslinked polystyrene based low-refractive index material were synthesized and used to fabricate the 1D PC sensor. As the model liquid analytes, hazardous volatile organic compounds benzene, toluene, and xylene were used in this study. The fabricated 1D PC sensor completely discriminated the benzene, toluene, and xylene as red, orange, and yellow-green colors, respectively, with showing high reflectivities (> 41%). In addition, the 1D PC sensor exhibited excellent reversibility and recyclability. These findings can be applied in developing high performance 1D PC sensors for detecting liquid analytes with high visibility and reliability.

Poster Presentation : **POLY.P-2**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Preparation and Characterization of Water-Soluble PPE Polymers and Their Potential Use

Nasim Sepay, Mohuya Paul[1], Jungkyun Im[1,*]

Department of Electronic Material and Devices Engineering, Soonchunhyang University, Korea

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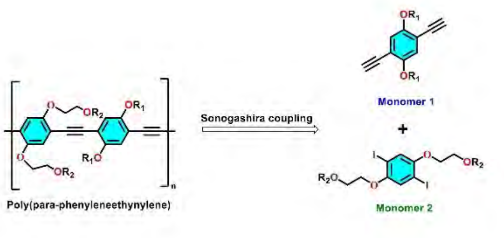
Recently researchers have put immense interest in effective sensing, imaging, and therapeutic strategies for the treatment of diseases by quick and accurate diagnosis. Among the various available techniques for sensing and imaging, the strategies based on fluorescence exhibit noticeable advantages and offer distinctive opportunities. Structurally improved conjugated polymers with hydrophilic and functional pendant substituents have shown great potential applications in many fields including fluorescence sensors due to their high sensitivity and selectivity of detection measurement. However, most reported conjugated polymers do not have appreciable aqueous solubility and functional moieties for sensing and delivery. Therefore, we have designed and synthesized a water-soluble conjugated polymer, poly(para-phenyleneethynylene), by the polymerization of Monomer 1 and Monomer 2 via Pd-catalyzed Sonogashira coupling reaction. The side chain alteration of the PPE with different functional groups can allow it to explicitly recognize targets like enzymes, DNA, etc. Therefore, these improvements make our synthesized PPE appropriate for sensing and imaging.


OR$_1$
Monomer 1
Sonogashira coupling
+
OR$_2$
R$_1$O
OR$_1$
n
R$_2$O
Monomer 2
Poly(para-phenyleneethynylene)

Poster Presentation : **POLY.P-3**

Polymer Chemistry

Event Hall FRI 11:00~13:00

High refractive index copolymer-titania hybridized material with controllable refractive index according to titania content

Minju Jeong, Tae Gyu Hwang, Min Jeong Choi, Jongnam Park[1,*], Jong-Mok Park[*]

Research Center for Advanced Specialty Chemicals, Korea Research Institute of Chemical Technology, Korea

[1]*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

High refractive index materials that have been widely used recently are inorganic materials and are easily brittle. As an alternative to this, highly stable polymeric optical materials have widely been developed. The refractive index of optical materials is one of the important properties. Polymer/inorganic hybridization have been utilized in increasing refractive index of polymers while maintaining varied advantages of the polymers. In this study, novel copolymer/titania hybridized materials with high refractive index were designed, and their refractive index change according to the titania content was investigated. Photo-crosslinkable poly(N-Isopropylacrylamide-co-dopamine acrylamide-co-4-benzoylphenyl acrylate) (P(NIPAM-co-DA-co-BPA)) containing a hydroxyl group was synthesized. The synthesized copolymer was hybridized with the titania using titanium n-propoxide. In addition, copolymer/titania hybrid Ti10, Ti30, Ti50, and Ti70 were synthesized by controlling the weight fraction of titania in the copolymer/titania hybrid. The synthesis of copolymer/titania hybrids was confirmed by FT-IR and TGA and their refractive indices were examined with spectroscopic ellipsometer. Although the refractive index of conventional polymers was relatively low than inorganic materials, copolymer/titania hybrid Ti70 exhibited high refractive index of 1.71. This result can provide significant insights in developing optical materials such as lens, mirror, etc.

Poster Presentation : **POLY.P-4**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Discrimination of Hydrocarbons (C6~C14) using Novel 1D Photonic Crystal Multilayer Sensor for The Identification of Adulterated Diesel Oil.

Min Jeong Choi, Jong-Mok Park, Tae Gyu Hwang, Minju Jeong, Sang-Il Choi[1,*], Seohyun Jung[2,*]

Research Center for Advanced Specialty Chemicals, Korea Research Institute of Chemical Technology, Korea

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[2]*Research center for advanced specialty chemicals, Korea Research Institute of Chemical Technology, Korea*

Recently, there has been a problem of selling fake diesel by mixing diesel and kerosene. The use of fake diesel can cause problems with car engines, which can eventually lead to accidents. Therefore, it is significantly important to discriminate the adulterated diesel in commercially available oil products. In this study, we developed hydrocarbon sensing 1D photonic crystal (1D PC) film for discriminating the difference between diesel and kerosene. For this, photo-cross-linkable poly(4-methylstyrene-co-benzophenone acrylate) (P(4MS-co-BPA)) and poly(octylacrylate-co-benzophenone acrylate) (P(OA-co-BPA)) were synthesized and used as a high-refractiveindex polymer and low-refractiveindex polymers, respectively. The 1D PC films were fabricated by alternately stacking the high/low-refractive-index polymers on a black poly(ethylene terephthalate) (PET) substrate. The fabricated 1D PC sensor was applied in discrimination of adulterated diesel oil, and it was confirmed that the color change rates of 1D PC sensor were differentiated depending on the mixing ratios of diesel and kerosene. Therefore, it was confirmed that the developed 1D PC film was suitable for the discrimination of adulterated diesel oils.

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Poster Presentation : **POLY.P-5**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Outstanding Thermal Stability of 1D/2A Terpolymer-based Polymer Solar Cells Processed with Nonhalogenated Solvent

Hyeonwoo Jung, Youngu Lee*

Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

Polymer solar cells (PSCs) using a bulk heterojunction (BHJ) have attracted attention because of their unique advantages such as lightweight, flexibility, and low cost. Single-junction PSCs based on the PM6 copolymer show good photovoltaic performance in single junction PSCs only when treated with a halogenated solvent such as chlorobenzene (CB) or chloroform (CF). However, PM6 copolymer-based PSCs processed with nonhalogenated solvents exhibit relatively low PCE due to undesirable morphological properties, including high aggregation, rough surface morphology, and unfavorable edge-on orientation. Recently, terpolymers consisting of three different monomers in the polymer backbone have emerged as promising p-type polymers. The incorporation of a third monomer into a D–A copolymer backbone can create numerous combinations that may have a synergetic effect on physicochemical properties such as miscibility, energy levels, charge-carrier mobility, and crystallinity. Herein, we synthesized a novel series of 1D/2A terpolymers (PBTPBD) with different ratio of benzo[1,2-b:4,5-b‘] dithiophene-4,8-dione, and thieno[3,4-c]pyrrole-4,6(5H)-dione for the development of high-efficiency and long-lived PSCs processed with ecofriendly nonhalogenated solvents. The PBTPBD-50:IT-4F PSC, processed with o-xylene, exhibited a high PCE of 13.64%, which is 13% higher than that of PM6:IT-4F PSCs. Furthermore, the PBTPBD-50:IT-4F PSC maintained 82% of the initial PCE even after 204 days at 85°C, which is the highest thermal stability ever achieved with a PSC processed with an ecofriendly nonhalogenated solvent.

Poster Presentation : **POLY.P-6**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Single-Cell Nanoencapsulation with Nature-Derived Eggshell Membrane Hydrolysates and Coffee Melanoidins

Sang Yeong Han, Gyeongwon Yun, Eunhye K. Kang, Beom jin Kim[1], Ji Hun Park[2], Insung Choi[*]

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[1] *Department of Chemistry, University of Ulsan, Korea*
[2] *Department of Science Education, Ewha Womans University, Korea*

A pair of eggshell membrane hydrolysates (ESMHs) and coffee melanoidins (CMs) has been utilized for layer-by-layer (LbL) construction of artificial exoskeletons in single-cell nanoencapsulation (SCNE). Hydrogen bonding-based LbL-SCNE of *Saccharomyces cerevisiae* is extremely cytocompatible (viability > 99%), and the ESMH/CM shell effectively protects the cells from various lethal stressors, such as heavy metals (Cd^{2+}, Cu^{2+}, and Zn^{2+}), pH fluctuation, and UV-B irradiation. The durability and cytoprotectability of the ESMH/CM shell are further enhanced by Fe^{3+}-mediated shell cross-linking.

Poster Presentation : **POLY.P-7**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Sustained release of Clonidine-loaded PLGA microspheres containing 1-hydroxy-2-napthoic acid

Jihyang Lim[*], ByungCheol Shin[1]

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[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Clonidine, an alpha-2 adrenergic agonist, is a drug for the treatment of tic disorder and attention deficit hyperactivity disorder (ADHD). In the previous study, O/W clonidine-loaded microspheres increased the loading efficiency compared to W/O/W clonidine-loaded microspheres, but showed an irregular drug release profile. Therefore, we developed clonidine-loaded PLGA microspheres with 1-hydroxy-2-napthoic acid for sustained release and zero-order release kinetics. The microsphere were prepared by O/W emulsion solvent evaporation method. The effects of various parameters such as polymer composition, the type of release retardant, the ratio of 1-hydroxy-2-napthoic acid and the drug content were confirmed. The physicochemical properties and drug release were evaluated through encapsulation efficiency, morphology of microspheres, drug distribution, thermal analysis and in vitro release study. As a result, the microspheres with lactic acid/glycolic acid ratio of 75:25 and 1-hydroxy-2-napthoic acid were suitable for zero-order release model. In addition, the drug release rate was delayed and the correlation coefficient (R^2) improved as the ratio of 1-hydroxy-2-napthoic acid was increased. Therefore, it is expected that clonidine-loaded PLGA microspheres with 1-hydroxy-2-naptoic acid are useful for treatment of tic disorder and ADHD for long periods.

Poster Presentation : **POLY.P-8**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Polarity sensing and nano-imaging of polymer film using spectrally resolved super-resolution imaging

Yejin Park, Doory Kim*

Department of Chemistry, Hanyang University, Korea

The increasing research attention on the rational design of material surfaces has led to the development of various functional polymer coating methods to obtain the aimed surface properties. Due to the importance of characterization of polymer surface in many areas of chemistry, such as adsorption and heterogeneous catalysis, the local measurement of the chemical properties of polymer nanostructures is of great significance. Among various chemical properties of the polymer surface, the surface polarity is considered important to understand the chemical performance of the polymer surface. Although various surface-specific measurement methods have been used to investigate the surface polarity of polymer film, they are not suitable to detect the heterogeneity in polymer coatings since they are ensemble-averaged macroscopic measurements. Here we developed a new optical approach to unveil the nanoscale structure and composition of various polymer films at the single-molecule level using our custom-built spectrally super-resolution microscopy. By simultaneously recording the super-resolution images and single-molecule emission spectra of individual solvatochromic molecules embedded inside or on the surface of various polymer films, we could map their nanoscale local polarity. Moreover, we successfully demonstrated the nanoscale demixing of polymer blend films based on the different polarity of polymer components using our novel method.

Poster Presentation : **POLY.P-9**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Poly[(1,1-dialkyl-3,4-diphenyl-2,5-silolene)-co-(ethynylene)] by the Stille Coupling Reaction of 2,5-Dibromosiloles with Bis(tributylstannyl)acetylene reagent and Electrochemical Characterization

Ji hun Lee, Young Tae Park*, Se Yeon Park[1], Hyeong Rok Si[1]

Department of Chemistry, Keimyung University, Korea
[1]*chemistry department, Keimyung University, Korea*

Dialkyl(R = Et, or *iso*-Pr, or *n*-Hex)-bis(phenylethynyl)-silanes were reacted with lithium naphthalenide, anhydrous zinc chloride, and *N*-bromosuccinimide (NBS) to obtain 1,1-dialkyl(R = Et, or *iso*-Pr, or *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles, respectively. Poly[(1,1-dialkyl-3,4-diphenyl-2,5-silolene)-co-(ethynylene)], conjugated polymers containing with silolene and acetylene, were synthesized through the Stille coupling reaction of 1,1-dialkyl-2,5-dibromo-3,4-diphenyl-siloles and bis(tributylstannyl)acetylene as co-monomers, in the presence of toluene as solvent and dichlorobis(triphenylphosphine)palladium as catalyst. The crude products were purified by precipitation with methanol and then furthermore purified by extraction with chloroform. The obtained polymeric materials were analyzed by ^{1}H, ^{13}C, ^{29}Si NMR, FT-IR, GPC and UV-vis spectroscopy. The electrochemical properties of the prepared polymers as anode materials for lithium-ion batteries was also studied. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

Poster Presentation : **POLY.P-10**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Oxidative Coupling Polymerization of 1,1-Dihexyl-2,5-diethynyl-3,4-diphenyl-silole

Se yeon Park, Young Tae Park*, Ji Hun Lee, Hyeong Rok Si

Department of Chemistry, Keimyung University, Korea

1,1-Dialkyl (R = Et, or *iso*-Pr, or *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles were prepared by the reactions of 1,1-dialkyl (R = Et, or *iso*-Pr, or *n*-Hex)-1,1-di(phenylethynyl)silanes with lithium naphthalenide, zinc chloride, and *N*-bromosuccinimide (NBS), respectively. Two bromine groups of the prepared siloles were substituted with two trimethylsilylethynyl groups using trimethylsilylacetylene (TMSA) under the solvent of diisopropylamine and catalysts such as palladium chloride, copper iodide, and triphenylphosphine, of which 1,1-dialkyl (R = Et, or *iso*-Pr, or *n*-Hex)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles were yielded, respectively. 1,1-Dihexyl-2,5-diethynyl-3,4-diphenyl-silole was only successfully prepared by desilylation reaction of 1,1-dihexyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-silole with potassium carbonate (K_2CO_3) and co-solvent of tetrahydrofuran (THF) / methanol. After the reaction was finished, potassium carbonate was removed by washing with dilute HCl aqueous solution. The crude product was extracted with dichloromethane (DCM), and further purified by recrystallization in hexane. 1,1-Dialkyl (R = Et, *iso*-Pr, *n*-Hex)-2,5-diethynyl-3,4-diphenyl-siloles were also successfully prepared by the reactions of 1,1-dialkyl (R = Et, *iso*-Pr, *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles with ethynylzinc chloride, of which was prepared in situ with reaction of ethynylmagnesium bromide with zinc chloride, and bis(triphenylphosphine)palladium(II) dichloride as catalyst. The obtained product was soluble in usual organic solvents such as tetrahydrofuran and dichloromethane. All the prepared materials were characterized by ^{1}H, ^{13}C, ^{29}Si NMR, IR, and UV-Vis spectroscopic methods. Oxidative coupling polymerization of 1,1-dihexyl-2,5-bis(ethynyl)-3,4-diphenyl-silole was also tried under the reaction condition of copper(I)chloride and amine/acetone as co-solvent with bubbling oxygen gas.
Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

Poster Presentation : **POLY.P-11**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis of 3-component acrylic copolymers and their adhesion properties in thin films

Hyewon Lee, WeonTae Oh*

Dong-Eui University, Korea

Recently, with the spread of COVID-19, the use of disposable products is increasing significantly, and the size of the disposable wipes market is also growing rapidly. The types and contents of alcohols used in wet wipes are increasing due to the need for disinfection and sterilization functions. As alcohols are used in wet tissue products, it is necessary to improve the physical properties of the adhesive sticker used for the wet tissue packaging cover. The existing adhesive stickers for the packages of wet wipes are low to the alcohol stability, causing destruction and swelling of the adhesive layer.In this study, to develop emulsion-type adhesive resins using water as a solvent, copolymers were synthesized with combinations of acrylic monomers 2-EHA, BAM, and LMA (or OA). In addition, a small amount of silicone acrylate was added and used to control adhesion and re-peelability with the substrate. The adhesive properties were characterized in terms of the monomer compositions of the synthesized acrylic copolymers and the contents of silicone acrylate. The adhesive properties and alcohol resistance of the synthesized copolymer adhesive were evaluated.

Poster Presentation : **POLY.P-12**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Facile Approach to Grafting Sulfobetaine Polymers on Solid Surfaces for Antifouling Applications

Inho Kim, Sung Min Kang*

Department of Chemistry, Chungbuk National University, Korea

Zwitterionic polymer grafting onto solid surfaces has been of special interest because it exhibits excellent antifouling property. Various studies have been conducted to achieve facile and robust grafting zwitterionic polymers onto solid surfaces, but previous studies showed limitations in that large amounts of reagents are required. Herein, a facile, coordination-driven approach to grafting sulfobetaine polymers on solid surfaces is developed. Sulfobetaine polymers with different molecular weights are synthesized and grafted on the polydopamine-coated surface via metal-mediated crosslinking reactions. The resulting surfaces show strong resistance to protein adsorption and marine diatom adhesion.

Poster Presentation : **POLY.P-13**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Application of fully optimized silver nanowire patterned electrodes to flexible polymer solar cells

Su Hong Park, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

We developed an effectively patterned silver nanowire(AgNW)-based electrode for application to flexible polymer solar cells (PSCs). The transparent poly(2-hydroxyethyl methacrylate) underlayer improved the adhesion between the flexible substrate and the AgNWs. The overcoat layer using PEDOT:PSS and a small amount of 2,4-hexadiyne-1,6-diol as a UV sensitizer addressed the issue of AgNW roughness and AgNW patterning ability. The optimized AgNW-based electrode showed a low sheet resistance of 22.6 Ω/□ and a transmittance of 92.3% at 550 nm. The corresponding flexible PSC exhibited a high PCE of 11.20%, similar to that of the PEN/ITO-based control device. In addition, the excellent mechanical stability of the AgNW-based device was confirmed through bending tests for up to 10,000 bending cycles at a bending radius of 6.0 mm. These results suggest an effective and excellent flexible electrode manufacturing method that can be applied to other electronic and optoelectronic flexible devices.

Poster Presentation : **POLY.P-14**

Polymer Chemistry

Event Hall FRI 11:00~13:00

New Hole Transport Polymers: Orthogonal solvent system for solution-processable organic light-emitting diodes

Hyeondoo Je, Dong Hoon Choi[1,*]

Chemistry, Korea University, Korea
[1]*Department of Chemistry, Korea University, Korea*

In the solution process OLED, when the top layer is formed, the layer already formed on the bottom is swollen or dissolved by the solvent of the top layer. To solve this problem, HTL and EML were formed using chlorobenzene and toluene, respectively. However, it is very difficult to develop a lower layer that is not soluble in toluene. This problem can adversely affect the efficiency of the device. Therefore, it is important to find a solvent that can dissolve the EML well without affecting the polymer HTL. In this study, a new green TADF-OLED device was fabricated as a multilayer structure using a different solvent system. In general, instead of forming ETL on HTL using toluene solvent, ETL was formed using a new solvent capable of dissolving only emitting materials. This device not only formed a good interface and enables efficient charge transport, but also showed a constant turn-on voltage and efficiency compared to the previously used chlorobenzene/toluene system.

Poster Presentation : **POLY.P-15**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Elongation Ratio of Stretchable PDMS Depending on the Molecular Weight of Polysiloxane

Young Ji Song*, Jihee Choi

Research Department, KNW Co., Ltd., Korea

Materials for stretchable display have been widely studied in recent years. Polydimethylsiloxane (PDMS) has big adventages of thermal stability, oxidation resistance, transparency under UV or light and moisture stablility. Studies on PDMS for stretchable display have been started because of these characteristics of polysiloxanes. PDMS shows diverse characters depending on the molecular weight, ratio and type of siloxanes and crosslinkers. The elongation ratio has increased as molecular weight of polysiloxane increases. In the case of crosslinker that has Si-H group on the main chain, elongation ratio has decreased as percentage of crosslinker increases. And which has Si-H group on the side chain, elongation ratio has increased as percentage of crosslinker increases.

Poster Presentation : **POLY.P-16**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Polymerization-Induced Nanostructuring of Janus Bottlebrush Polymers

Changsu Yoo, Myungeun Seo*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Polymerization-induced nanostructuring strategies such as polymerization-induced self-assembly (PISA) and polymerization-induced microphase separation (PIMS) are efficient routes to produce block copolymer nanoparticles and nanostructured block copolymer materials. Nanostructuring spontaneously occurs during polymerization in situ as the segregation strength of the forming block copolymer exceeds the onset of microphase separation. Here we explore the effect of Janus bottlebrush polymer architecture in the self-assembled morphologies induced by polymerization. We will investigate the influence of the backbone length on the segregation strength and the morphology to understand how the Janus bottlebrush backbone can pre-program and rigidify the interface.

Poster Presentation : **POLY.P-17**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Graphite-mediated Synthesis of Fluorenylidene Bis(2-phenoxyethanol) for High Refractive Index Optical Resin

Ju-Young Choi, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Optical materials use optical properties such as light transmittance, fluorescence, and light concentration. The components constituting these include lenses, prisms, reflectors, etc. We focused on lenses. In the past, glass lenses were used a lot in camera lenses, but now plastic lenses with many advantages in formability, weight, and mass production are being used. FBPE [fluroenylidenebis(2-phenoxyethanol)] is used as a monomer for plastic lens polymers.In the existing method for synthesizing FBPE, 9-fluorenone and 2-phenoxyethanol are used as reagents. The reaction conditions are the high temperature of about 60 ℃ for sulfuric acid and mercaptopropionic acid. At this time, use four equivalents of 2-phenoxyethanol compared to Fluorenone, and use mercaptopropionic acid, which is harmful to the human body. We improved these parts in three ways: 1. Reducing the equivalent of 2-phenoxyethanol, 2. Using Graphite as an alternative catalyst without using mercaptopropionic acid, and 3. Reducing the reaction temperature.

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Poster Presentation : **POLY.P-18**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Characteristics of Phosphorescent Organic Light-Emitting Devices with p-type Conjugated Polymer Hole Injection Layers

Sooyong Lee, Hwajeong Kim, Youngkyoo Kim*

Department of Chemical Engineering, Kyungpook National University, Korea

Organic light-emitting devices (OLEDs) have recently been a major player in display industries through gradual innovations of organic semiconducting materials and device structures. Most OLED displays with small and medium sizes have been fabricated by thermal evaporation processes of individual small molecules for each color sub-pixel in devices. In terms of large-size OLED displays for television sets, color filters (including color conversion films) for basic colors (red, green and blue, for example) are attached on the front of common white OLED backlit parts that are fabricated via the similar thermal evaporation processes of small molecules in vacuum. These vacuum processes are expensive and limit the size of OLED displays, which motivated wet-coating processes of soluble organic materials including conducting polymers. In this presentation, we shortly report that solution-processed nanolayers of p-type conjugated polymers can act as an efficient hole injection layer for phosphorescent OLEDs.

Poster Presentation : **POLY.P-19**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Mechanochemical Synthesis of Polyurethane from CO_2-Captured Biomass-derived Polyols and Their Application to Composite Materials with High Thermal Conductivity

Inhwan Cha, **Eun Joo Kang**[1,*], **Changsik Song**[*]

Department of Chemistry, Sungkyunkwan University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Because of the environmental issues associated with thermoset polymers, recyclable polymers are highly in demand, and the use of sustainable biomass-derived ingredients is also becoming increasingly important. Also, As the degree of integration of electronic devices is improved, the development of a heat control material generated is also required. In this work, we synthesized thermoset polyurethane (CPU) from carbon dioxide and biomass-derived monomers via a facile, solvent-free ball milling process. In addition, it was possible to produce a highly dispersed polyurethane-based hybrid composite material by PU polymerization with a thermal filler through the ball milling process. Synthesized CPUs may have transcarbamolyation, which is one of dynamic covalent bond exchanges. Taking advantage of this chemistry, we proposed that the CPU based composites were expected that the interfacial thermal resistance between the heat-sink and the heat source at high temperature would be lowered. Dynamic mechanical thermal and stress relaxation analyses indicated that the NPU films possess typical characteristics of vitrimers, such as constant crosslink density and Arrhenius-like reduction in viscosity at elevated temperatures, even though the dissociative exchange of urethane bonds may work here. Also, CPU-based hybrid materials were confirmed with high thermal conductivity through laser flash analysis (LFA). Our mechanochemical approach is facile and scalable, enabling the preparation of sustainable and recyclable polymers and hybrid composites.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **POLY.P-20**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Photogenerated Charge-Aided Low-Voltage Operation of n-Channel Organic Transistors

Seungmok Lee, Hwajeong Kim, Youngkyoo Kim*

Department of Chemical Engineering, Kyungpook National University, Korea

Organic field-effect transistors (OFETs) have drawn keen attention because of various advantages over conventional inorganic FETs in terms of low-temperature solution processes, flexible and foldable shapes, etc. However, the charge carrier mobility of OFETs is still far behind a commercial level. As an alternative way, the OFET studies have been broadened toward a low-current device such as photodetectors, temperature sensors, chemical sensors, tactile sensors, etc. Another challenge in OFETs is to reduce the operating voltages that are correlated with the charge mobility of organic semiconducting materials. Recently, our group tried to utilize photons as a core mean to make effective channels in OFETs that cannot be operated at low voltages. In this presentation, we report the possibility of photogenerated charge-aided operation of n-channel OFETs at low voltages.

Poster Presentation : **POLY.P-21**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Poly(L-Alanine-co-L-Lysine)-g-Trehalose As a Biomimetic Cryoprotectant for Stem Cells

Zhengyu Piao, Hyun Jung Lee, Jinkyung Park, Byeongmoon Jeong*

Department of Chemistry and Nano Science, Ewha Womans University, Korea

Poly(L-alanine-co-L-lysine)-graft-trehalose (PAKT) was synthesized as a natural antifreezing glycopolypeptide (AFGP)-mimicking cryoprotectant for cryopreservation of mesenchymal stem cells (MSCs). FTIR and circular dichroism spectra indicated that the content of α-helical structure of PAK decreased after conjugation with trehalose. Two protocols were investigated in cryopreservation of MSCs to prove the significance of the intracellularly delivered PAKT. In protocol I, MSCs were cryopreserved at -196 oC for seven days by a slow cooling procedure in the presence of both PAKT and free trehalose. In protocol II, MSCs were preincubated at 37 oC in PAKT solution, followed by cryopreservation at -196 oC in the presence of free trehalose for seven days by the slow cooling procedure. Polymer and trehalose concentrations were varied, respectively. Cell recovery was significantly improved by protocol II with preincubation of the cells in the PAKT solution. The recovered cells from protocol II exhibited excellent proliferation and maintained multi-lineage potentials into osteogenic, chondrogenic, and adipogenic differentiation, similar to MSCs recovered from cryopreservation in the traditional dimethyl sulfoxide 10% system. Ice recrystallization inhibition (IRI) activity contributed to cell recovery, however intracellular delivered PEG-PAKT was the major contributor to the enhanced cell recovery in protocol II. Inhibitor studies suggested that macropinocytosis and caveolin-dependent endocytosis are the main mechanism for intracellular delivery of PEG-PAKT. Dynamic light scattering and 1H-NMR spectra suggested that the intracellular PEG-PAKTs interact with the cell membrane and intracellular components, which might contribute to stabilize the cells during cryopreservation.

Poster Presentation : **POLY.P-22**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Study of thermal stability in ternary blended organic solar using highly miscible semiconducting polymer

Sangah Park, **Daehwan Lee**[1], **Taiho Park**[2,*]

Chemical Engineering, Pohang University of Science and Technology, Korea
[1]*Pohang University of Science and Technology, Korea*
[2]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*

The thermal stability of organic solar cells (OSCs) is still crucial requirement for photovoltaic technology. Tailoring morphology of blend system is a key factor of power conversion efficiency (PCE) and thermal stability of OSCs. Herein, we synthesize a novel asymmetric NDI-based polymer (asy-PNDI1FTVT) and demonstrate a multi-functional OSC with PTB7-Th/Y6 blend system. Owing to the asymmetric structure of asy-PNDI1FTVT, the resulting ternary blend system shows lower crystallinity than symmetric polymer (PNDITVT, PNDI2FTVT) based blend systems in 2D grazing-incidence wide-angle X-ray scattering (2D-GIWAXS) results. Since low crystalline property of asy-PNDI1FTVT forms a well-intercalated morphology at the PTB7-Th:Y6 blend system, the PTB7-Th:Y6: PNDI1FTVT device facilitates efficient charge dissociation with enhanced fill factor (FF) and PCE. Resultingly, ternary system of PTB7-Th:asy-PNDI1FTVT:Y6 showed a PCE of 12.5%, suppressing the phase separation of blend system with negligible burn-in loss (at 75 °C for 400 h).

Poster Presentation : **POLY.P-23**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Supramolecular Phthalimide Networks via Diels-Alder Reaction-Aromatization Approach with Biomass-derived Furanic Dienes

Byounghyun Kim, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Polyurethane (PU) is a major engineering material with excellent heat resistance and rubber-like elasticity, mostly synthesized from petroleum-based resources which lead to environmental pollution. Furfuryl materials can be easily obtained from lignocellulose, which can be applied as a sustainable material such as biomass-derived polymer platforms. This eco-friendly platform can be used to form supramolecular gels or network polymers, and its physical properties can be controlled through the Diels-Alder (DA) reaction. In this study, a carbamate group was introduced directly at the C-2 position in furan. By increasing the HOMO energy level due to the electron-donating effect, this structure showed an improved DA reaction rate compared to the structure in which substituted a methylene group. In addition, a supramolecular gel is formed through intermolecular interaction between DA adducts, which has a different gelation rate due to the conformation according to various maleimides. Based on this, we intend to form a supramolecular gel that responds to anions by introducing polyol. If the formed supramolecular gel responds to harmful anions (e.g. cyanide, phosphate, and nitrate) in the air, it is expected that it can be used in the field of eco-friendly sensors.

Poster Presentation : **POLY.P-24**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Single-Ion Conducting Polyether Electrolyte via Orthogonal Post-Polymerization Modification

Jiyoung Lee, **Byeong-Su Kim***

Department of Chemistry, Yonsei University, Korea

The substitution of organic liquid electrolytes with solid-state electrolyte has been regarded as an alternative for overcoming the safety issues of lithium-ion batteries (LIBs). Among diverse solid-state electrolytes, poly(ethylene oxide) (PEO)-based polymer electrolytes feature high flexibility and ion solvating ability albeit with its relatively low ionic conductivity at room temperature due to semicrystallinity. To overcome this challenge, the present study presents the polyether-based single ion conducting polymers that can simultaneously tune various properties of solid-state electrolytes, including ion conductivity and mechanical properties. Specifically, a series of polyether was synthesized through epoxy-amine bulk polymerization using the reaction between diepoxide and amine derivatives. From this platform, a pendant side chains retaining either oligo(ethylene glycol) groups and bulky anionic groups were further introduced by orthogonal post-polymerization modification. This strategy not only improves the segmental motion, but also increases the contribution of lithium cations to the total current, which can contribute to the improvement of ionic conductivity. In addition, the feasibility of this approach for LIBs was evaluated by analyzing the dielectric properties and ionic conductivity of the resulting polymers.

Poster Presentation : **POLY.P-25**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Ring-opening alternating copolymerization of cyclic anhydrides and functional epoxides by using organic Lewis pair catalysts

Sumin Lee, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

Ring-opening alternating copolymerization of cyclic anhydrides and epoxides has been considered a promising strategy that are capable of producing tailor-made polyesters with a great variety of structures, functionalities, and properties. Herein, we synthesized polyesters bearing carboxylic acid pendants using a cyclic anhydride and a novel functional epoxide monomer, *t*-butyl glycidoxy acetate (*t*-BGA), followed by acidic deprotection. A Lewis pair catalyst comprising a mild phosphazene base, *t*-BuP$_1$, and triethylborane, Et$_3$B, was first optimized for the polymerization of diglycolic anhydride (DGA) and *t*-BGA to yield the polyesters of P(DGA-*alt*-*t*-BGA) with a controllable molecular weight and dispersity. As a control, glutaric anhydride (GA) was used to polymerize the P(GA-*alt*-*t*-BGA). The resulting polymers were characterized via ^{1}H- and ^{13}C-NMR, GPC, DSC, and MALDI-ToF analyses. Interestingly, the effect of oxygen heteroatoms in cyclic anhydrides on the properties of polyesters with carboxylic acid pendants was found to exhibit a significant influence on the physical and chemical properties of the resulting polyesters.

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Poster Presentation : **POLY.P-26**

Polymer Chemistry

Event Hall FRI 11:00~13:00

N-Triflyl Phosphoric Triamide (N-TPT) based Quartz Crystal Microbalance Chemical Warfare Agent Sensor

Sun Gu Song, Changsik Song[*], Han yong Bae[*]

Department of Chemistry, Sungkyunkwan University, Korea

We designed and synthesized the N-TPT receptors which is a novel triple hydrogen bonding donor molecules for CWA detection via non-covalent host-guest interactions. The highly robust trifurcate molecular structures were designed based on density functional theory (DFT) computations and synthesized from phosphorous (V) chlroride via simple stepwise procedure. The synthesized receptors were coated on the QCM sensors by simple drop-casting method and CWA simulant DMMP was measured. The sips isotherm model was fitted to the concentration dependent responses and calculated results. From the results, we revealed the mechanism of detection and could obtain the higher sensitivity toward DMMP than previously reported receptors and selectivity to other volatile organic chemicals (VOCs).

Poster Presentation : **POLY.P-27**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Highly efficient and oxygen-tolerant visible-light-curing acrylic resins for UV-absorbing adhesives of foldable displays

Daewhan Kim, Min Sang Kwon*

Department of Materials Science and Engineering, Seoul National University, Korea

Flexible electronics have emerged as a key future technology enabling a variety of astonishing new applications such as flexible lighting and displays, wearable sensors for health monitoring, implantable electronics for medical diagnosis and treatment, soft robotics, and conformable energy harvesting devices. Conventional adhesives used at a display are optically clear adhesives (OCAs) that are prepared by UV-light curing of acrylic resins. Since UV-absorbing OCAs contain additives with a strong UV-light absorption, which prevents photoinitiators (PIs) absorbing UV-light, they cannot be prepared by the conventional photocuring method. We therefore envisioned that the development of new acrylic resins that are effectively cured upon irradiation by visible light would provide a great solution. Furthermore, the system would be more beneficial to address the inherent issues of the current UV-curing system, for example, oxygen sensitivity. We fabricated UV-absorbing adhesive via exquisitely designed visible-light curing system with excellent efficiency and oxygen-tolerance. Various photocatalysts (PCs) and sacrificial reductants were screened to find best combination that facilitates good conversion in acrylic bulk polymerization. Finally, using 4Cz-IPN and hybrid-reductants (DMAEAc and DMAEA) exhibited best performance showing fast initiation of polymerization and adjustable crosslinking degree to be used for foldable smartphone in the presence of limited amount of oxygen. The optimized adhesive showing excellent curing behavior under UV blocking condition can be used for not only OCA but also the application area of the PC-based adhesive to foldable display.

Poster Presentation : **POLY.P-28**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Controlled micropore in hyper-cross-linked polymer via in-situ removal of porogenic templates

Wonjune Yeo, Myungeun Seo*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Microporous polymers with pores smaller than 2 nm have high potentials for separations, heterogeneous catalysis, and gas storage. Hyper-cross-linked polymers (HCPs) have been one of the most widely investigated and commercialized microporous polymers. However, the amorphous nature of the randomly cross-linked network has limited fine-tuning of pore size that can enable size-selective adsorption of guest molecules. Herein, we present a synthetic approach to control the micropore size by incorporating porogenic groups that can be removed during the hyper-cross-linking reaction. The effect of the porogenic group size will be discussed along with the synthetic and characterization details.

Poster Presentation : **POLY.P-29**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Principal Components of Self-healing Nanofiber-based Time-temperature Indicator for Cold-chain Systems

Semin Kim, Hye Kyeong Sung, Jeyoung Park*

Center for Bio-based Chemistry, Korea Research Institute of Chemical Technology, Korea

Public interest in cooking and food has increased the supply of groceries and meal kits. Accordingly, the importance of the cold chain system for transporting food and the storage environment is increasing. To visualize food exposure to a high-temperature environment, an irreversible time-temperature indicator (TTI) could be utilized. In our previous work, we developed a nanofiber TTI based on self-healing behavior. To expand the usability for various conditions, we developed TTIs with different specifications. Interestingly, it was possible to fabricate TTIs which has discrete healing time without any changing the components and ratio of the self-healing material.In the resin synthesizing procedure, we conduct a 2-step reaction: 1) diisocyanate with polyol, and 2) the resultant 1) with chain extender. In the 1st step, diisocyanate injection time and the initial concentration of the polyol (degree of dilution in reaction solvent) affect the viscosity of the product polymer solutions. The viscosity is the key factor that determines the self-healing time of TTIs. In this work, we find out the correlation between the variables and the healing time of TTIs in various environments.

Poster Presentation : **POLY.P-30**

Polymer Chemistry

Event Hall FRI 11:00~13:00

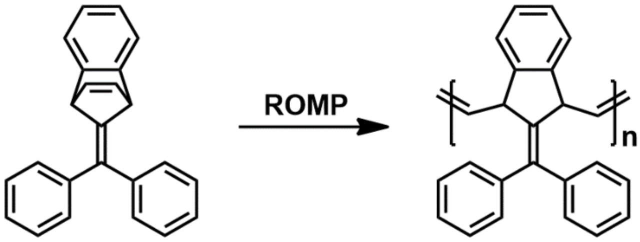
Synthesis of Stable Benzonorbonadiene Polymers via Ring-opening Metathesis Polymerization

Huijin Lee, **Cheoljae Kim**[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea

[1]*Department of Chemistry, Chungbuk National University, Korea*

We have synthesized an air-stable poly(benzonorbornadiene) polymers via ring-opening metathesis polymerization. Due to the unstable benzylic/allylic hydrogen, the poly(benzonorbornadiene) polymers are easily decomposed by oxidation, and two avoidances have been reported either by reducing the allylic double bond or by substituting the allylic hydrogen. We demonstrated stable poly(benzonorbornadiene) polymers by hiding unstable benzylic/allylic hydrogen with structural steric bulky aryl side groups. Further research on the application of conjugated polymer synthesis are ongoing.



Poster Presentation : **POLY.P-31**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Critical chiral bias for the decision of supramolecular chirality upon coexisting internal and external chiral information

Jun Su Kang, Dong Ki Yoon, Mi Hee Lim, Woo youn Kim[1], Myungeun Seo*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, KAIST, Korea*

Life on earth has evolved to have homochirality by favoring only one enantiomer of the mirror-image pair. Such prevailing single chirality has been attributed to the symmetry breaking from the racemic state in the prebiotic stage followed by transfer and amplification of the asymmetry into the mesoscopic and macroscopic levels through hierarchical self-assembly. Circularly polarized light (CPL) is considered a possible origin of the slight chiral bias that could have produced homochirality by asymmetric photochemical reaction. While some recent papers report direct induction of chiral information in CPL to the supramolecular assemblies from the achiral systems, the impact of incident CPL during the evolution of supramolecular chirality in presence of molecular chirality has remained elusive. Here, we clarify the mechanism of the light-induced asymmetric self-assembly by using chiral and achiral triarylamine derivatives. We explore the emergence of supramolecular chirality resulting from cooperative or competitive interactions by matching and mismatching their handedness. Finally, the critical chiral bias that can determine handedness of supramolecular chirality will be quantitatively evaluated. This work will provide insights into the light-matter chirality transfer and designing multiscale chiral systems.

Poster Presentation : **POLY.P-32**
Polymer Chemistry
Event Hall FRI 11:00~13:00

Thermoplastic Elastomers Prepared by Renewable Resources from Lignin and Fatty Oils

Soyeon Kim, Haneul Kim, Sumin Lee, Byungjin Koo[*]

Department of Polymer Science and Engineering, Dankook University, Korea

Thermoplastic elastomers (TPEs) are composed of triblock copolymers with hard chains on each side and soft chains in the middle. One of the most widely utilized TPEs is poly(styrene-b-butadiene-b-styrene), or SBS. Since it is often prepared from petroleum-based monomers, great efforts have been put in order to replace them with renewable resources. In this work, we designed a new type of TPE wherein monomers can be potentially obtained from depolymerized lignin building blocks that serve as hard chains and fatty alcohols that serve as soft chains. Specifically, for a hard block, we used phenyl acrylates which are known to be prepared from lignin (from trees) depolymerization (leading to phenol) and subsequent acrylation. For a soft block, we employed n-octyl acrylates that can be prepared from fatty alcohols (vegetable oils) and subsequent acrylation. Using these monomers, we applied the reversible addition-fragmentation chain-transfer (RAFT) polymerization using trithiocarbonate derivatives as a chain-transfer agent. With this agent, phenyl acrylates were first polymerized, followed by the copolymerization with n-octyl acrylates. Although the polymerization was successful (Mn 86,000 g/mol, PDI 1.60), we observed the low glass transition temperature (Tg) of phenyl acrylate blocks at 24 ℃. To achieve TPE-like properties, we are currently optimizing the polymer structures to increase the Tg by adjusting hard blocks with phenyl acrylate and styrene, followed by the polymerization of soft blocks.

Poster Presentation : **POLY.P-33**

Polymer Chemistry

Event Hall FRI 11:00~13:00

1-D hypo-crystal: A step towards equilibrium crystallization of polycarbonate

Thanh Van Vu, Youngjong Kang*

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It is known that stretched extended chains polymer was the most stable form of polymer crystal, however, typically polymer chains are not stretched out that during conventional polymer crystallization, they form folded lamellae since the chains quickly fluctuate back to their coiled state before they can effectively interact with other extended chains. Poly(bisphenol-A carbonate) (PC) is a widely used amorphous polymer due to its high impact resistance, transparency, thermal stability and good electrical properties. While the theoretical equilibrium melting temperature of PC is known as T^0_m = 318 ºC, most of reported crystallization methods provide much lower values, implies that most of PC crystallites are far from the ideal equilibrium stretched structure. Herein, we report crystallization of PC by thermal quenching of PC using benzoic acid (BA) as the stretching agent. After BA removal, PC exhibited a clear endothermic melting transition at T_m = 225 ºC. The PC crystals exhibited characteristic features of 1-D crystals structure that one dimension was laterally packed (d = 4.1 and 3.4 Å) independently from chain conformation while the other two dimensions were still amorphous due to the randomness of *trans-trans* and *trans-cis* conformation in PC backbone chain. Surprisingly, the melting point sharply jumped to the higher temperature, T'_m = 285ºC upon annealing at 180 ºC for a few hours, which was attributed to the crystalline transition. The new melting point was closer to the equilibrium melting temperature, while taking much shorter time than previous researches.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Development of fully bio-based epoxy polymers with photo-driven self-healing property

Jiyun Kim, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

In this study, we designed a novel epoxy network polymer with an epoxy monomer obtained from a dimer acid, which can be easily obtained from vegetable and animal oils and photo-reactive plant-derived trans-cinnamic acid. It is expected to be a very eco-friendly route in that it does not use toxic catalysts and solvents. In addition, the C=C bond moiety of the synthesized epoxy polymer is expected to be beneficial for the formation of a self-healable network via photo-induced [2+2] cyclization reaction.

Poster Presentation : **POLY.P-35**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Analyzing Gamma-Ray Irradiation Effects of Polystyrene/SW-CNT composites

DaeHee Lim, Ha Eun Shim, Byoung-Min Lee, YouRee Nam, Yeong Heum Yeon, Jungho Mun, Jae Yeon Park, Jaehyun Lee, Moonsik Chae, Hui-Jeong Gwon*

Radiation Reaction Model Research Lab, Korea Atomic Energy Research Institute, Korea

Nowadays, the commercial polymers are becoming more important in industries and in our daily life. Because they have many advantages such asdiverse functionality, low cost, lightweight, ease of processing and excellent chemical stability. Over the past few decades, many researchers have found some changes in structural, optical, thermal and electrical characteristics of these commercial polymers under irradiation conditions. Moreover, the incorporation of carbonnanotubes (Single-Walled Nanotubes, SW-CNTs) into polymers can change their own properties of both two materials. In addition, many of the reported papers describe theoretical and experimental studies of various diameter-dependent properties of CNTs. Thus, for systematic study, the SW-CNTs with the different diameters are introduced into the polystyrene to improve radiation resistance and other properties. In this study, we demonstrate polystyrene/SW-CNTs composites with various diameters SW-CNTs to check the property changes including radiation protective characteristics under various dose of gamma radiation conditions.

Poster Presentation : **POLY.P-36**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Impact of Mechanical Force Transfer on Spiropyran Activation

Chae Won Lee, Chiyoung Park[1,*]

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[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Mechanophore is a class of molecules that contains a part that mechanically responds to external stimuli. Generally, spiropyran can be converted into merocyanine form under mechanical force because of weak C-O bond, which can generate color and fluorescence change. This characteristic of spiropyran linked to the bulk polymer has the advantage of visualizing the mechanophores activation. Until now, many studies are focused on the direct force applied to spiropyran in a polymer matrix. In this work, we study the isomerization of spiropyran by indirect force through rotaxane end-capped with spiropyran.

Poster Presentation : **POLY.P-37**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Controlled Synthesis of Various Low-Bandgap Donor-Acceptor Alternating Conjugated Polymers via Suzuki-Miyaura Catalyst-Transfer Polymerization

Hwangseok Kim, Tae-Lim Choi[*]

Division of Chemistry, Seoul National University, Korea

Donor-acceptor alternating conjugated polymers (D-A ACPs) are potent organic semiconducting materials for organic light-emitting diodes, organic field-effect transistors and polymer solar cells. However, to date, precision synthesis of D-A ACPs with controlled molecular weight and narrow dispersity had limited scope due to the lack of a synthetic method. Herein, we report that Suzuki-Miyaura catalyst-transfer polymerization (SCTP) using RuPhos-Pd catalyst is an advantageous platform for controlled polymerization of various D-A biaryl monomers. With this SCTP method, four D-A CPs (PBTzEDOT, PQXTh, PQXEDOT, PQXSe) were obtained with controlled molecular weight, narrow *Đ*, and high yield (>87%). In addition, the SCTP operated even on a quateraryl monomer with carbonyl functionality to give a A_1-D-A_2-D terpolymer (PBTzThDPPTh) in a chain-growth manner, highlighting the excellent ring-walking ability of RuPhos-Pd as well as high functional group tolerance of SCTP. Notably, the D-A ACPs showed different optical (E_g^{opt} from 1.29 to 1.77 eV) and electrochemical (HOMO level from -5.57 to -4.75 eV) properties depending on the electronic characters of D/A units. Furthermore, living nature of the SCTP realized the one-pot synthesis of unprecedented di- and triblock copolymers having complex microstructures (D-DA, A-DA, DA-DA and A-D-DA).

Poster Presentation : **POLY.P-38**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Dual stimuli-responsive viologen-containing poly(2-alkyl-2-oxazoline) hydrogel

JeongMin Lee, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Viologen-containing thermo-responsive poly(2-alkyl-2-oxazoline) (**POx-2V^{4+}**) was designed as a responsive-functional materials. During the cationic ring opening polymerization, living chain end was reacted with hexaethylene glycol having 4,4'-bipyridyl end groups to produce thermo- and redox-responsive **POx-2V^{4+}**. An aqueous solution of **POx-2V^{4+}** showed decreasing in transmittance upon increasing the temperature through the hydrophilic-hydrophobic phase transition. When sodium dithionite was added to the solution of **POx-2V^{4+}**, the transparent solution was immediately changed to a violet colored solution, indicating the formation of a stacked radical cation by single-electron reduction (**POx-2(V^{2+})$_2$**). As increasing temperature of the violet solution, **POx-2V^{4+}** turns blue and opaque by aggregation of polymer (**POx-2V^{2+}**). The blue color was slowly covered to transparent by aerobic oxidation. The same changes in transmittance and color in response to temperature and redox environment, respectively, were observed in hydrogel state.

Poster Presentation : **POLY.P-39**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Unusual Regioselectivity in Cycloaddition of Aziridine Achieved by Polymer Mechanochemistry

Suin Choi, Sangmin Jung, Lee Kangsik, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Regioselectivity is of importance to syntheses of small molecules, polymers, and nanomaterials. This presentation shows that polymer mechanochemistry enables unusual regioselectivity that cannot be achieved under the traditional conditions. Specifically, upon ultrasonication, N-phenolic aziridine embedded into a macromolecular backbone undergoes C-N bond scission to afford the corresponding azomethine ylide, which subsequently reacts with a dienophile, dimethyl acetylenedicarboxylate (DMAD), and produces exclusively 2-pyrrolidine derivative. By contrast, the analogous reaction under thermal conditions yields a positional isomer, 3-pyrrolidine derivative. Our work demonstrates an unprecedented synthetic route to generate a positional isomer that cannot be produced under traditional thermal conditions.

Poster Presentation : **POLY.P-40**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Cascade Cyclopolymerization of 5-ethynyl-1,8-nonadiyne to Synthesize Conjugated Polyacetylenes Containing Fused Bicyclic Ring Unit and Their Optical Properties

Hanseul Ryu, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

The cyclopolymerization via olefin metathesis is a powerful method to synthesize the functional polyacetylene. Using this method, polyacetylenes containing various ring sizes ranging from four-membered to seven-membered rings have been synthesized. However, the repeat unit structure was limited to mono cycloalkene because conventional cyclopolymerization used diyne monomers, and any attempt to change this backbone structure was unprecedented. Herein, we demonstrate novel cascade cyclopolymerization, which involves sequential olefin metathesis of rationally designed triyne derivatives with three terminal alkynes to change the backbone structure to a fused bicyclic ring. In addition, we can control the regioselectivity by altering the catalyst structure and synthesize polymers containing fused bicyclic [4,3,0] or [4,4,0] units with high molecular weight (up to 119 kDa). Interestingly, obtained polymers showed improved optical properties (e.g., narrower bandgap) compared to polymers with mono cycloalkene units in the backbone due to the planarization of conjugated segment result from fused bicyclic ring structure.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Characterization of Fluorosilicone Resins Using Cyclic Fluorosilane Compounds

Hansan Ko, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

1,3,5-tris[(3,3,3-trifluoropropyl)methyl]cyclotrisiloxane, referred to as FD3, is used as a precursor for many high molecular weight compounds. In this study, a resin was synthesized through a simple process of ring-opening and polymerization of FD3, and a water-repellent coating solution was prepared and evaluated using FD3 resin. The synthesized resin was analyzed for physical properties through Si-NMR and GPC, and a water-repellent coating solution was prepared by mixing it with fluorosilicone. It was confirmed that the coating solution in which the two materials were properly mixed had the highest water contact angle compared to the coating solution using only FD3 and the coating solution using only fluorosilicone.

Poster Presentation : **POLY.P-42**

Polymer Chemistry

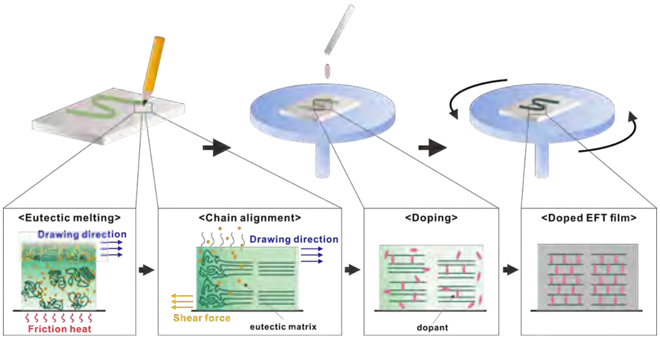
Event Hall FRI 11:00~13:00

A Charge-Transfer Doping of P3HT film by Eutectic Friction Transfer Method with F4TCNQ

SangWon Eom, Ngoc Bao Tran[1], Youngjong Kang[*]

Department of Chemistry, Hanyang University, Korea
[1]*Chemistry Department, Hanyang University, Korea*

An eutectic friction transfer (EFT) is based on the eutectic melting by frictional heating at the interface between the pellet made of semiconducting polymer/matrix mixture and the substrate. Due to the significantly lowered melting temperature by formation of eutectic mixtures (< 65 °C), various semiconducting polymers can be easily melted and transferred on the substrate simply by rubbing the pellet on the substrate. in this case, semiconducting polymer chains can be uniaxially aligned and crystallized by the frictional shear force. Futher, we combined eutectic friction transfer with charge-transfer doping. The uniaxially aligned P3HTEFT film was obtained from the eutectic friction transfer method, and F4TCNQ-doping was conducted to the P3HTEFT film. F4TCNQ-doped P3HTEFT film shows highly anisotropic characteristics. P3HT polarons are uniaxially aligned along the P3HT chains, and F4TCNQ anions are perpendicularly located to the P3HT polarons. The F4TCNQ-doped P3HTEFT film was analyzed by polarized UV-vis and IR spectrometer



Poster Presentation : **POLY.P-43**

Polymer Chemistry

Event Hall FRI 11:00~13:00

High-Modulus and High-Osteoconductive Acrylic Bone Cement by Impregnating Hypo-crystalline PMMA Powder and Bioactive Glass 45S5

Myung Soon Hwang, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

The poly(methyl methacrylate) (PMMA), the mainstream substance used for commercial acrylic bone cement (ABC), has intrinsic characteristics such as biocompatibility, easy processability, and high mechanical strength. This study substituted pristine PMMA powder with hypo-crystallized-PMMA(hc-PMMA) powder and bioactive glass 45S5. The unique nanostructure and high modulus of the hc-PMMA itself have enhanced the compressional strength of the resulting bone cement. Due to the increased surface area and internal strain formed by the crystallization process, the addition of hc-PMMA dramatically decreased the polymerization time without any additional catalyst. Finally, the resulting bone cement showed higher osteoconductivity than the conventional ABC composite, which was confirmed by the simulated body fluid (SBF) test. Based on the results, hc-PMMA and bioactive glass 45S5 incorporated bone cement can be an optimal candidate for the long-term fixation of the load-bearing implants.

Poster Presentation : **POLY.P-44**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Electro-Mechanochemically Controlled Reversible Release of Guest Molecules from Metal-Phenolic Nanovalve and Its Hybrid Assemblies

Gyeonghyeon Choi, Chiyoung Park*

Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

Recently, there are several outstanding developments of therapeutic and drug delivery systems such as microchips, micropumps, and soft devices with sensor. However, the use of a battery and complicated preparation limits their implantable and wearable applications. Therefore, we report facile preparation of hydrogel matrix with the reversible nanovalve in response to electrical, ultrasound, electromechanical, and triboelectric stimuli. This research can suggest that the efficient platforms for active-type drug delivery applications based on implantable gels and transdermal patches with remotely controllable release characteristics.

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Mechanical properties of PBMANa ionomers

Kwang-Hwan Ko, Joon-Seop Kim[1,*]

Department of Biochemical & Polymer Engineering, Chosun University, Korea

[1]*Department of Polymer Science and Engineering, Chosun University, Korea*

The dynamic mechanical properties of poly(butyl acrylate-co-sodium methacrylate)(PBMANa) ionomers were measured and compared with styrene ionomers and methyl methacrylate ionomers having sodium methacrylate units. It is observed that in the case of PBMANa ionomer, with increasing ion content, the peak position of the matrix loss tangent was not changed and the height of the matrix loss tangent peak decreases. These results were different from those obtained from the styrene ionomers. This difference is probably due to the difference in the polarity and stiffness of main chain of styrene and butyl acrylate.

Poster Presentation : **POLY.P-46**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Mechanical properties of PBMANa ionomers containing PLA compounds

Kwang-Hwan Ko, Joon-Seop Kim[1,*]

Department of Biochemical & Polymer Engineering, Chosun University, Korea

[1]*Department of Polymer Science and Engineering, Chosun University, Korea*

The effects of the addtion of poly(lactic acid)(PLA) on the dynamic mechanical and thermal properties of poly(butyl acrylate-co-sodium methacrylate)(PBMANa) ionomers were studied using DMA, TGA, DSC techniques. It is also compared with styrene ionomers containing PLA. It is observed that the PLA increased the matrix peak height without changing the ionic modulus and the matrix peak positon of PBMANa ionomers with increasing the PLA amounts.

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Poster Presentation : **POLY.P-47**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Physical properties of 3-components acrylic copolymer prepared by aqueous emulsion polymerization

Kihun Lee, Youngmin Kim[*], WeonTae Oh[1]

S&H ELIZA, Korea

[1]*Dong-Eui University, Korea*

Disposable wet wipes, which have been increasingly used in recent years, are almost recognized as necessities in daily life. As the demand for disinfecting wipes containing antibacterial ingredients such as alcohol has increased due to the spread of COVID-19 over the past few years, the packaging specifications and the demanding properties of wet tissue products are also changing. Unlike conventional wet wipes, disinfectant wipes contain a high alcohol content, so the adhesive sticker for general wet wipes cannot be used.In this study, we develop acrylic pressure-sensitive adhesives of water-based emulsion type that can satisfy environmental friendliness while ensuring chemical resistance, interfacial adhesion, and re-peelability of adhesive stickers against alcohol components. The 3-components hybrid copolymers are prepared with 2-EHA, acrylic rubber based on the acrylic monomers, and silicone. The adhesive properties and alcohol resistance of the copolymers are characterized. For the adhesive properties, 180o peel test, heat resistance retention, and ball tack are measured according to ASTM D3330 standard. In the case of adhesion, it had high values of 500 gf or more, resulting in good interfacial adhesion. In the alcohol-resistance test, it was confirmed that the contents were stably kept in the package.

Poster Presentation : **POLY.P-48**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Elongated Cascade Enyne Metathesis Polymerization: Investigation of Stereochemistry and Structure Effect

Eunsong Jung, Tae-Lim Choi[1,*]

Department of chemistry, Seoul National University, Korea
[1]*Division of Chemistry, Seoul National University, Korea*

Cascade metathesis reaction is an efficient way to prepare multiple rings in a single step. Recently, we reported a polymerization of sugar-based monomers by controlled cascade enyne metathesis, which delivers decomposable macromolecules. In order to explore the principle of this system in a more complex monomer, we extended the enyne relay system by introducing an additional cycloalkene ring in the monomer. Herein, we report a study of the synthesis of monomers containing a terminal alkyne and two cycloalkene rings and their controlled polymerization, as described by a linear relationship between molecular weight and monomer-to-initiator ratio. Moreover, we developed a polymer decomposition protocol to accurately assess the degree of cascade efficiency and investigated how stereochemistry or structural modifications affect the cascade efficiency. In these monomers' structures, we observed *anti* stereochemical relationships, higher ring strain of the secondary cycloalkene, and larger substituents proximal to the alkyne head enhance the cascade efficiency.

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Event Hall FRI 11:00~13:00

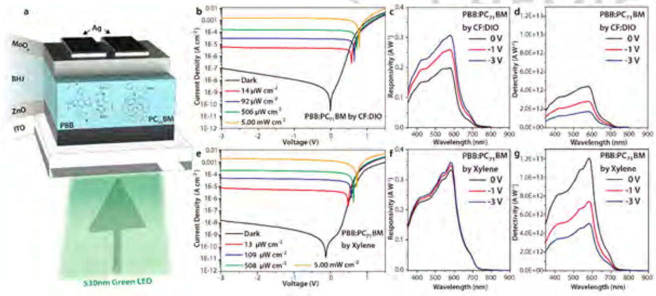
New conjugated polymer layered rapidly response organic photodetector using non-halogen solvent

WonJo Jeong, **Cheol Shin**[1], **In Hwan Jung**[1,*]

Department of organic and Nano Engineering, and Human-Tech Convergenece Program, Korea

[1]*Department of Organic and Nano Engineering, Hanyang University, Korea*

The new polymer (4-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b'] Dithiophen-2-yl)-2,6-dioctylbenzo[1,2-d:4,5-d']bis(oxazole)) (PBB) shows a rapid response and the synthesis method is facile. PBB monomer is benzobisoxazole, it is synthesized three steps and don't have column chromatograpy at final product. PBB polymer has good solubility, so it dissolves in xylene, a non-halogen solvent. Responsity, detectivity, and signal response time were measure in chloroform, a halogen solvent, and xylene, a non-halogen solvent. It was measured to be R of 0.385 A/W and specific detectivity (D*) 1.33 × 10^{13} Jones (at –1 V), 3 μs in xylene and R of 0.349 A/W and D* of 5.86 × 10^{12} Jones at (–1 V), 42 μs in chloroform. Acceptor is used as PCMB, and in Xylene, PBB and $PC_{70}BM$ are stacked as if they made layers. And then PCBM was adjacent to ZnO, charge and transport dynamic properties were improved.



Poster Presentation : **POLY.P-50**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Donor-Acceptor Type Conjugated Copolymers in a Continuous Flow Reactor

Youngrok Kim, Jin Woo Jun, Ye-Jin Hwang*

Department of Chemistry and Chemical Engineering, Education and Research Center for Smart Energy and Materials, Inha University, Korea

Continuous flow reactor is a powerful synthetic technique to overcome some chronic issues in the reactions using traditional batch reactors. Donor-acceptor (D-A) type conjugated polymer is a promising material for the future devices by having attractive properties such as flexibility, light weight, low cost, as well as easy processing. Traditionally they have been synthesized in a batch reactor. However, it is hard to avoid several issues represented by batch-to-batch variation, a phenomenon in which polymers have different material properties and causes ununiform device performance. On the contrary, the use of continuous flow reactor can provide a large-scale, safe, and controllable synthesis of donor-acceptor type conjugated polymers in a highly reproducible manner. In this work, we synthesized six D-A type conjugated copolymers chosen by paring well-known repeating units, including naphthalene diimide (NDI), benzodithiophene (BDT), and diketopyrrolopyrrole (DPP). The polymers were synthesized in various reaction conditions, and the molecular weight was successfully tuned. Thus, we believe that we demonstrated the great potential of flow synthesis system to replace conventional batch system.

Poster Presentation : **POLY.P-51**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Reproducible and rapid synthesis of a conjugated polymer by Stille polycondensation in flow: Effects of reaction parameters on molecular weight

Chanseo Lee, Seungjun Lee, Ye-Jin Hwang*

Department of Chemistry and Chemical Engineering, Education and Research Center for Smart Energy and Materials, Inha University, Korea

Conjugated polymers are promising material which can be applied in various devices such as organic photovoltaics(OPVs), organic field-effect transistors(OFET) and light emitting diodes(LEDs). However, in the batch synthesis system which is used widely for conjugated polymer synthesis, batch-to-batch variation occurs leading uncontrolled molecular weight and irreproducible device performance. Flow synthesis system can be an excellent alternative to batch synthesis system by providing rapid and reproducible reactions. Flow system effectively transfers heat and mass, so it enables uniform reaction and high reproducibility. In our study, we developed a flow system using nitrogen gas as a carrier instead of pure solvent or fluorinated oils to eliminate the common diffusion problems at the beginning and the end of the reaction stream to the carrier fluid. Without the diffusion problem, our system provides high reproducibility and uniform reaction conditions in all regions of reaction stream. Using our system, PTB7, one of the most representative conjugated polymers, was synthesized to highlight performance of our flow system. We found that PTB7 with a number average molecular weight (Mn) over 30 kDa was synthesized in only 3 min, with very low deviations of 2.6% and 3.1% for Mn and Đ values, respectively, compared to deviations of 66% for Mn and 43% for Đ in control reactions using pure solvent as a carrier. The effect of catalyst loading and reaction temperature was also studied, which enabled tuning the Mn of PTB7 within the range of 30.6–57.9 kDa. The quality of PTB7 synthesized in our system was also confirmed by fabricating photovoltaic devices which gave maximum power conversion efficiency of 7.02% with PC71BM as an acceptor.

Poster Presentation : **POLY.P-52**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Effect of ozonized graphitic nanofibers on fracture toughness of carbon fiber/epoxy composites

Seong-Hwang Kim, Soo-Jin Park[1,*]

Chemistry, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

A graphitic nanofiber (GNF) surface was successfully modified using the dry-ozone treatment for use as the reinforcement for carbon fiberreinforced composites (CFRPs). To evaluate the efficacy of the proposed method, CFRPs are fabricated at different weight contents along with two other types of composites. We denoted the specimens of GNF/CF/ epoxy composites and OGNF/CF/epoxy composites as GCE and OGCE composites, respectively. The mechanical properties including ILSS and KIC were studied for composites to evaluate their efficiency. The measured highest ILSS and KIC value reached 34.2 MPa and 55.4 MPa.m1/2 in the OGCE composites, equating to enhancements of 22.6 and 14.2% compared to the GCE composites.

Poster Presentation : **POLY.P-53**

Polymer Chemistry

Event Hall FRI 11:00~13:00

High Performance All Polymer Photodetector via Control the Molecular Structure of Small Molecule Acceptor

Jinhyeon Kang, Hyeokjun Kim[1], Doyeong Yeo[2], In Hwan Jung[*]

Department of Organic and Nano Engineering, Hanyang University, Korea
[1]*Hanyang University, Korea*
[2]*Organic & nano engineering, Hanyang University, Korea*

There are two strategies to increase the polymer-based photodetector (PPD) performance. One strategy is to increase the wavelength selectivity, and the other strategy is to increase the photodetective properties such as responsivity (*R*) and specific detectivity (*D**). However, many studies for PPDs mention that there is a trade-off relationship between wavelength selectivity and photodetective properties. In order to improve both properties, we newly designed small molecule acceptor (SMA) which exhibited asymmetric molecular structure and similar absorption wavelength with polymer donor material. The high miscibility between polymer donor and SMA induced the increased *R* and *D** values of 0.31 A/W and 2.0×10^{13} Jones at -2 V under 532 nm LED illumination, respectively. Also the fabricated device exhibited relatively narrow full width at half-maximum (FWHM) of 230 nm.

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Poster Presentation : **POLY.P-54**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Antimicrobial Hydrogels: pH-driven Release of Bioactive Aldehyde from Triblock Copolyether Hydrogels

Neha Choudhury, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

Microbial disease, as a terrible natural alarm, has turned into a worldwide health risk and tormented humanity for a long time. Clinically significant antibacterial resistance posed a worldwide threat in the 21st century. As one of the solutions, antimicrobial hydrogels can offer high microbial inhibition ability, hydrophilicity, cell adhesion capability, biocompatibility, and more interestingly, their degradability can be tailored by altering temperature, ionic strength, pH, and light. Herein, we synthesize polyether-based ABA triblock copolymer hydrogels bearing poly(ethylene oxide) (PEO) midblock and a hydrophobic end-block wherein the bioactive aldehydes with potential antimicrobial activity were affixed *via* pH-responsive acetal linkage. Initially, a series of triblock copolymers were fabricated *via* anionic ring-opening polymerization of functional epoxide monomer with varying the end-block degree of polymerization. Upon dissolution in water above a critical polymer concentration, the triblock copolyethers generated the hydrogels. Triggered release of the bioactive aldehydes from the hydrogels was achieved in acidic pH through the hydrolysis of acetal pendants which resulted in a dynamic gel-to-sol transition. Coupled with its high biological activity, the antimicrobial hydrogel developed in this study will offer a new means for the treatment of microbial disease.

Poster Presentation : **POLY.P-55**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Effect of amine-treated graphitic nanofibers on fracture toughness of epoxy nanocomposites

Seong-Hwang Kim, **Soo-Jin Park**[1,*]

Chemistry, Inha University, Korea

[1]*Department of Chemistry, Inha University, Korea*

In this work, the amino-functionalized graphitic nanofibers (TGNFs) are successfully modified using a tetraethylenepentamine to use as a reinforcement in epoxy composites. To validate the interfacial interaction between the GNF and epoxy, composites are fabricated using three different types of GNF, namely the bare GNF, the acid-treated GNF (AGNF), and the TGNF, each with various GNF contents. The optimal GNF loading for the bare and AGNF is shown to be 0.50 wt.%, while that of the TGNF is as high as 0.75 wt.%. The highest fracture toughness values of 25.8 MPa.m1/2 are demonstrated for the TGNF-loaded composites with the fraction of 0.75 wt.%, representing enhancements of ~400%, respectively, compared to those of the neat composites.

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Poster Presentation : **POLY.P-56**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Effect of dry-carboxylated microcrystalline cellulose on interfacial properties of epoxy nanocomposites

Seong-Hwang Kim, Soo-Jin Park[1,*]

Chemistry, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

In this study, microcrystalline cellulose (MCCs) were treated with HNO3/H2SO4. MCCs were observed for surface properties using FT-IR and X-ray photoelectron spectroscopy and were used in the epoxy composites. In addition, the fracture resistance of the epoxy-based nanocomposites was investigated by measuring the fracture toughness (KIC). The related reinforcing mechanisms were also analyzed, and the enhancements on fracture resistance was mainly be attributed to interfacial interlocking effect.

Poster Presentation : **POLY.P-57**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Polymer Mechanochemistry with Ball-Mill Grinding

Jinkyung Noh, Ye-Jin Hwang[1], Tae-Lim Choi, Gregory Peterson[2,*]

Division of Chemistry, Seoul National University, Korea
[1]*Chemical Engineering, Inha University, Korea*
[2]*Chemistry, Incheon National University, United States*

Ball-mill grinding (BMG) has become an important method for conducting solid-state polymer mechanochemistry. We have studied the influence of various BMG parameters and polymer properties on the rates of mechanochemical chain scission events, including the activation of mechanophores. Specifically, the glass transition temperature has been found to be an important parameter which influences the degradation rates of linear amorphous polymers. Furthermore, polymer architecture has also been found to have a drastic influence, and provides an important set of parameters for tuning the mechanochemical reactivity of polymers.

Poster Presentation : **POLY.P-58**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Improvement strategy of PbS quantum dot-based NIR photodetectors via introducing π-conjugated polymers as a hole transporting layer

<u>MyeongIn Kim</u>, Gyuri Kim, Jaehee Park, In Hwan Jung*

Department of Organic and Nano Engineering, Hanyang University, Korea

As the demand for near-infrared (NIR) detection increases in the fields of military industry, communications and medical health, how to develop high quality and low cost NIR photodetector has been grown attention. PbS colloidal quantum dot (PbS CQD) is one of the good candidate for the active material of optoelectronics due to its unique properties such as easily tunable bandgap, high absorption efficiency and so on. In typical PbS CQD-based optoelectronics, 1,2-ethanedithiol (EDT) treated PbS CQDs have been used for the hole transporting layer (HTL). In this work, we introduced benzodithiophene (BDT)-based conjugated polymers as a HTL in order to enhance the device performance through the increased hole mobility and morphological properties than those of EDT treated PbS CQDs. The optimized device with conjugated polymer HTL exhibited improved responsivity (R) and specific detectivity (D*) under 940 nm illumination.

Poster Presentation : **POLY.P-59**

Polymer Chemistry

Event Hall FRI 11:00~13:00

A simple screening method for the isolation of plastic-degrading bacteria

Giyoung Shin, Jeyoung Park[1,*]

Korea Research Institute of Chemical Technology, Korea

[1]*Center for Biochemistry, Korea Research Institute of Chemical Technology, Korea*

Synthetic plastics are deeply linked to daily lives. Plastics have made significant contributions to humanity through their excellent processability, mechanical properties, and low cost. However, plastic wastes are causing serious pollution as it accumulates in the ecosystem as a result of resistance to the environment. To accelerate the decomposition of plastics, it is necessary to identify efficient plastic-degrading microorganisms. Indeed, screening for these microorganisms is time-consuming and labor-intensive. It is a difficult task to distribute hydrophobic plastics with a high surface area and cell accessibility in a microbe culture medium in a uniform manner.In this study, we developed a rapid and facile micro-spray-based screening method for the isolation of plastic-degrading bacteria. Plastic microparticles are sprayed on a solid medium by an easy-to-use air spray apparatus, thereby providing a translucent screening plate. Micro-sprayed plastic particles share a large interface with microorganisms. The degrading activities of bacteria make a translucent region turn into a transparent zone around the colony. Visual changes according to degradation appear, enabling intuitive selection of plastic-degrading microorganisms.

Poster Presentation : **POLY.P-60**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Development of multi-crosslinked Chitosan/Urushi composite electrolyte

Jun Tae Kim, Jongok Won*

Department of Chemistry, Sejong University, Korea

Chitosan obtained from the deacetylation of chitin has non-toxic, biocompatible and biodegradable properties, and is a natural polymer that is easy to chemically modify because it has hydroxy groups and amino groups as functional groups. However, when making electrolyte materials with Chitosan like this, there are many limitations in material development due to poor mechanical properties compared to excellent ion conductivity. To reduce these disadvantages, this experiment introduced natural Urushiol with excellent durability and developed Chitosan/Urushi composite material. In order to increase interaction with Urushiol, a Catechol group was introduced by adding 3,4-dihydroxybenzaldehyde to chitosan. The Catechol group introduction and substitution rate was confirmed through IR and NMR. Various molar ratios of Chitosan/Urushi composite materials were prepared, and the combination of modified Chitosan and Urushiol was confirmed by FT-IR. The thermal properties of the composite electrolyte material were analyzed through TGA, and the mechanical strength of the membrane was measured through a tensile strength test. Electrolyte properties were confirmed by measuring ionic conductivity with EIS.

Poster Presentation : **POLY.P-61**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis of urushi organogel using vanadium.

Minseok Kim, Jongok Won[1,*]

Chemistry, Sejong University, Korea
[1] *Department of Chemistry, Sejong University, Korea*

Demand for natural polymers is increasing as the influence of synthetic polymers on the environment or ecosystem increases. As a natural polymer capable of replacing the physical properties of synthetic polymers, durability and chemical stability are high, and natural urushiol having a catechol group capable of introducing various functional groups is highly applicable in various fields. Urushiol undergoes an oxidation reaction by enzymes, heat, catalysts, etc., followed by polymerization to synthesize urushi polymers. Using the oxidation/polymerization reaction characteristics of natural urxiol, urushiol in a specific organic solvent may obtain urushiol having high mechanical strength due to chemical and coordinate bonds by Fe3+. In this study, urushi organogel by vanadium ions was synthesized and its characteristics were measured. Various concentrations of urushiol/--butyrolactone solutions were prepared, gelation conditions according to vanadium/urushiol molar ratio were found, and characteristics were analyzed by IR and rheology. The effect and correlation of Fe3+ and vanadium ions on gelation on urushi organogel were compared and analyzed.

Poster Presentation : **POLY.P-62**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Study of radiation-induced degradation with Geant4 simulation on PLDLA films as degradation models

Ha Eun Shim, Yeong Heum Yeon[1], YouRee Nam[1], DaeHee Lim[2], Byoung-Min Lee[1], Moonsik Chae[1], Jungho Mun[1], Jae Yeon Park[3], Jaehyun Lee[1], Hui-Jeong Gwon[4,*]

Radiation Reaction Model Research Lab., Korea Atomic Energy Research Institute, Korea
[1]*Korea Atomic Energy Research Institute, Korea*
[2]*Radiation Research Division, Korea Atomic Energy Research Institute, Korea*
[3] *방사선연구부, Korea Atomic Energy Research Institute, Korea*
[4]*Department of Chemical Engineering & Biotechnology, Korea Atomic Energy Research Institute, Korea*

Biodegradable polymers have recently been widely used as materials for medical devices. Among the various materials, poly(L-co-D,L lactide) (PLDLA) is very valuable materials used in medical applications as implantable devices because of their excellent flexibility and biodegradability. In this study, biodegradable PLDLA was evaluated using Geant4 (G4EmStandardPhysics_option4) for damage simulation to predict the safety of against gamma ray sterilization. To verify the simulation results, the physicochemical changes in the irradiated PLDLA films were characterized by GPC, ATR-FTIR, and DSC analyses. The Geant4 simulation curve for radiation-induced damage on molecular weight was consistent with the experimentally obtained results. This study is a preliminary study for radiation damage analysis and prediction of biodegradable polymers by gamma rays. In the future, it is expected to be used not only for radiation sterilization but also for simulator development research that can predict the optimal irradiation dose to ensure material decomposition safety in the processing process.

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Poster Presentation : **POLY.P-63**
Polymer Chemistry
Event Hall FRI 11:00~13:00

Synthesis of Sulfur Rich Nano- and Microparticles through Polymerization by Phase Transfer Catalysis

Yu Jin Jeon, Jeewoo Lim*

Department of Chemistry, Kyung Hee University, Korea

Sulfur-containing materials exhibiting intriguing properties such as high refractive indices and high electrochemical capacities have attracted keen interest in recent years for their utility in optical, pesticidal, and electrochemical applications. Sulfur rich polymer particles in processible form are expected to expand the scope of the application of sulfur-containing materials. Previous research on the interfacial polymerization of aqueous alkali metal polysulfides in the presence of a cationic surfactant, which played a dual role as a phase transfer catalyst, allowed for the preparation of well-defined sulfur-rich polymer particles with diameters ranging from 100 to 400 nm. Herein, we report the synthesis of sulfur rich nanoparticle from aqueous alkali metal polysulfides through the use of both a polymeric stabilizer and a phase transfer catalysts. Sulfur-rich polymer particles with diameters ranging from 360 nm to 1.2 μm were obtained and the size of the particles could be controlled by varying the concentration of the neutral surfactant.

Poster Presentation : **POLY.P-64**

Polymer Chemistry

Event Hall FRI 11:00~13:00

[Withdrawal] Synthesis of Poly(N-vinylcarbazole)-based p-Type Materials for Organic Light-Emitting Diodes

YoungSeung Ko, Bonju Koo, Hyejin Na, Jaemin Lee*

Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea

- Withdrawal -

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Poster Presentation : **POLY.P-65**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Preparation of Highly Fluorinated Block Copolymers through Ring-Opening Metathesis Polymerization.

Yohan Chang, Jeewoo Lim*

Department of Chemistry, Kyung Hee University, Korea

Fluorinated polymers exhibit a unique set of properties consisting of high thermal stability and high chemical resistance with intrinsically low surface energy. Fluorinated polymers also have low dielectric constants and can be applied to millimeter wavelength fifth-generation(5G) communications. These remarkable features are closely related to the polymer's overall fluorine content. Compounds with fluorine contents above 60 wt% in the form of long perfluoroalkyl chains are known to form their own “fluorous” phase. However, polymerization of high-fluorine content monomers is restricted due to their poor solubility and phase separation. PFOA is a typical surfactant used in polymerization of fluorinated polymers such as PVDF, PTFE, and PHFP. Nowadays, the use of PFOA has been restricted as it can accumulate in the body and exhibit serious animal-based toxicity. Polymer based fluorosurfactants, therefore, deserve merit. In this work, a series of diblock copolymers containing fluorine-rich blocks, prepared through ring-opening metathesis polymerization, are reported. The surfactants show good dispersibility in common organic solvents and can be utilized as surfactants for the dispersion of polymerization of fluoropolymers in non-fluorinated solvents.

Poster Presentation : **POLY.P-66**

Polymer Chemistry

Event Hall FRI 11:00~13:00

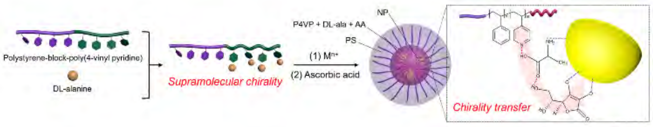
A General Route to Synthesize Chiral Inorganic Nanostructures from Achiral Platforms: Block Copolymer Template-Based Strategy

Minju Kim, **Yu Jin Jang**[1,*], **Dong Ha Kim**[*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea

[1]*Convergence Research Center for Energy and Environmental Sciences, Sungkyunkwan University, Korea*

Chiral inorganic nanostructures have attracted growing attention due to their potential applications and technological prospects. Even though various strategies have been developed for fabricating chiral inorganic nanostructures, the complex processes and expense of chiral biomolecules and their derivatives remain formidable challenges to realize mass production and large-area fabrication with simple and cost-effective processes. Here, we report a simple but generalized route for the synthesis of diverse chiral inorganic nanoparticles (NPs) such as Au, Ag, PdO, and TiO_2 NPs using achiral block copolymer (BCP) templates. Self-assembled BCP inverse micelles offered a specific environment for the evolution of chirality, where DL-alanine induced the left-handedness via hydrogen bond with pyridines of polystyrene-block-poly(4-vinyl pyridine). BCPs were then used as a chiral host to transfer its handedness to the anchored metal or metal oxide NPs, leading to an anisotropy factor of -8.6×10^{-4} for Au NPs. This value is higher than that obtained from the other chiral inorganic nanostructures fabricated based on helical polymer templates. Our design concept pinpoints forwarding steps to construct an extended library of viable chiral nanostructures, ensuring a substantial development of artificial chiral materials.



Poster Presentation : **POLY.P-67**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Formation of 2D Nanosheets with Tunable Size via Living CDSA of Conjugated Homopolymer

NamKyu Yun, Tae-Lim Choi[1,*]

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Semi-conducting 2D nanostructures, prepared by self-assembly of conjugated polymers, are promising materials for optoelectronics applications. Since the properties of these nanomaterials are size-dependent, there have been numerous efforts to control their size, shape, and dimensions. However, controlled self-assembly of conjugated polymers is still challenging due to their low solubility, especially for conjugated homopolymers without solubilizing shell block. Herein, we synthesized a polyenyne containing fluorene moiety by using living metathesis and metallotropy (M&M) polymerization with different degrees of polymerization. We could determine that such polymers have enhanced solubility compared to polyacetylene. Therefore, living crystallization-driven self-assembly (CDSA) of pristine polyenyne homopolymers could be achieved for the formation of uniform 2D nanosheets. Additionally, precise size-control could be achieved (from 0.6 μm^2 to 3.3 μm^2) by tuning the unimer-to-seed ratio.

Poster Presentation : **POLY.P-68**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Concentration dependent behaviors of PEG macromers in solutions and gels

Jungju Ryu[*], **Daewon Sohn**[1,*]

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This study aims to reveal how to describe the networks of poly(ethylene glycol) (PEG) gels with correlation length parameters. Polymer chains can produce networks at the concentration above overlapping concentrations, c*, where the correlation lengths exhibit the remnant structure in initial gel states. Here, we explored the concentration-dependent behaviors of liner and star PEG chains through dynamic light scattering and small-angle scattering measurements. The hydrodynamic radii and correlation lengths of star macromers decreased with the concentrations. The reduction magnitudes of the sizes change between the semi-dilute and dilute regimes, determining c*. It was observed that the correlation lengths at c* correspond to that in gels. On the other hand, the linear PEG produced cluster-like behaviors. The results provide the analysis method based on valid parameters that describe polymer gels.

Poster Presentation : **POLY.P-69**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Polymeric Hole-transporting Materials via Buchwald-Hartwig Amination and Their Application to Perovskite LEDs

Hyejin Na, Bonju Koo, Hyeon Woo Jeong, Jaemin Lee*

Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea

Palladium-catalyzed cross-coupling reactions such as the Suzuki-Miyaura and Stille reactions are conventional synthetic methods that enable the syntheses of many diverse triarylamine analogs. However, coupling partners for those reactions need specific functional groups, and thus, it restricts designing novel structured polymers. In this study, we report the development of two novel hole-transporting materials (HTMs; HTM-1 and 2) for perovskite light-emitting diodes (LEDs). These materials were synthesized by the Buchwald-Hartwig coupling reaction via direct cross-coupling reaction on amine group. The new HTMs had good thermal stabilities and suitable highest occupied molecular orbital (HOMO) levels as hole-transporting layers for perovskite LEDs. The basic chemical and physical properties of the new HTMs were thoroughly investigated by using NMR, GPC, UV-Vis spectroscopy, AC-2 and etc. Furthermore, a series of LED devices with different HTLs including PTAA, HTM-1 and HTM-2, have been fabricated and characterized. Comparable device characteristics were obtained when HTM-1 was applied as a HTM to red perovskite quantum-dot (QD) LEDs compared with PTAA. Besides green perovskite QD LEDs using HTM-2 showed approximately 1.4 times enhanced EQE compared to that using PTAA.

Poster Presentation : **POLY.P-70**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Sequence-Dependent Multiblock Copolymerization-Induced Self-Assembly

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Sequential block copolymerization in a selective medium can spontaneously induce self-assembly of the forming block copolymers by aggregation of the solvophobic blocks. In this polymerization-induced self-assembly (PISA) framework, extending the polymer chain multiple times with chemically distinct blocks is expected to produce unique complex morphologies as the polymerization-induced structural transition occurs within the pre-defined micellar structure. Here we explore multiblock copolymerization in the PISA condition by varying the block sequence. The polymerization-induced micellization behavior and the morphological evolution during the chain extension will be discussed in detail.

Poster Presentation : **POLY.P-71**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Enhancing Beta Phase of Polyvinylidene Fluoride by Thermal Decomposable Additive

Jinwoo Choi, Youngjong Kang[1,*]

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The beta-phase formed PVDF is well-known for its excellent ferroelectric, piezoelectric, and pyroelectric properties. In this work, the beta-phase structure of PVDF film and fiber is enhanced by adding Butadiene Sulfone. The samples are fabricated by using solution casting, spin coating, and wet spinning with incorporation of varying butadiene sulfone fractions. After fabrication, residue of the butadiene sulfone can be eliminated with vacuum oven. X-Ray diffraction, GI-WAXS and FT-IR are used to study the crystalline nanostructure of PVDF sample. The surface of the polymer is measured through scanning electron microscope(SEM). The measurement about its electroactive property is carried out to compare general PVDF sample with the butadiene sulfone added PVDF sample

Poster Presentation : **POLY.P-72**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Converting Imine into Benzoaxzole-linked Covalent Organic Framework

Jiwon Kim, Jong-Beom Baek*

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Effective conversion of unstable linkages to stable linkages is important for high stability and crystallinity of covalent organic frameworks (COFs). In this work, an unstable imine-linked COF was converted through post-oxidative cyclization to a stable aromatic benzoxazole-linked COF (BO-COF). The structure of BO-COF was assessed by Fourier-transform infrared, Solid-state nuclear magnetic resonance spectroscopy, Powder X-ray diffraction patterns, Transmission electron microscopy and nitrogen adsorption-desorption isotherms. The resulting COF derived from this efficient post-oxidative cyclization exhibited excellent chemical and thermal stability with high crystallinity. This approach can be broadly utilized for the synthesis of stable fused-aromatic COFs, widening materials applications.

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Poster Presentation : **POLY.P-73**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Effect of ambient plasma-treatments on thermal conductivity and fracture toughness of boron nitride nanosheets-reinforced epoxy composites

Won-Jong Choi, Soo-Jin Park[1,*]

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With the rapid growth in the miniaturization and integration of modern electronics, the dissipation of heat that would otherwise degrade the device efficiency and lifetime is a continuing challenge. In this respect, boron nitride nanosheets (BNNS) are of significant attraction as fillers for high thermal conductivity nanocomposites due to their high thermal stability, electrical insulation, and relatively high coefficient of thermal conductivity. Herein, the ambient plasma treatment of BNNS (PBNNS) for various treatment times is described for use as a reinforcement in epoxy nanocomposites. The PBNNS-loaded epoxy nanocomposites are successfully manufactured in order to investigate the thermal conductivity and fracture toughness. With these enhancements, the increases in surface free energy and wettability of the PBNNS/epoxy nanocomposites are shown to be attributable to the enhanced interfacial adhesion between the filler and matrix. It is demonstrated that the ambient plasma treatments enable the development of highly dispersed conductive networks in the PBNNS epoxy system.

Poster Presentation : **POLY.P-74**
Polymer Chemistry
Event Hall FRI 11:00~13:00

Characteristic studies of enhanced functional magnetic halloysite nanotubes for dye adsorption capacity at different pH conditions

Quang Nguyen Ngoc, Daewon Sohn[1,*]

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[1]*Department of Chemistry, Hanyang University, Korea*

The synthesis method of magnetic halloysite nanotubes (mHNTs) is obtained by immobilizing halloysite nanotubes and the mixture of FeCl2/FeCl3 via one-pot synthesis and multi component reactions (MCR). SEM, TEM, XPS, XRD characterizations are used to determine the surface morphology and Fe3O4 bonding structure inner and outer of nanotubes in acidic and basic environment. FT-IR, UV–vis, BET, and VSM analyze the chemical bonding and performance of the adsorbents with the appearance of magnetic nanoparticles in several aspects of adsorption capacity and magnetization. The effect of organic-inorganic hybridization provided the as-obtained adsorbents with uniform structure, superior pore structure, large specific surface area, and superparamagnetic properties. The composites halloysite/Iron oxide is an excellent candidate in dye adsorbing materials in which the magnetic are easily separated by the external magnetic This study will focus on enhancing the uniform of magnetic nanoparticles on pristine halloysite nanotubes through MCR. Also, the dye adsorption of the material will be measured for cationic dyes as methylene blue, Rhodamine B and sunset yellow at different pH conditions. These modified mHNTs exhibited high adsorption efficiency in the order of sunset yellow > methylene blue > Rhodamine B in acidic condition. The anti-anion interference capability laying on the exterior lumen of mHNTs for the removal of different dyes were also determined at different pH, which demonstrated that the nanofibrous adsorbents were widely reusable and suitable for several environments.Keywords: halloysite nanotubes, magnetic nanoparticles, adsorbent, dye adsorption, cationic dye

Poster Presentation : **POLY.P-75**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Internal structure of hydrogel containing laponite and temperature responsive poly(N-isopropylacrylamide)

Younhee Jeong, Daewon Sohn*

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Poly(N-isopropylacrylamide) (PNIPAM)-based hydrogels have wide applications with their unique thermo-sensitivity around lower critical solution temperature (LCST) of 32℃ close to the body temperature. NIPAM particles are highly swollen at room temperature, and particles shrink sharply when heat above the LCST. In this study, laponite-PNIPAM hydrogels were synthesized with different concentrations of clay. In the swelling test, the hydrogels showed a dramatic absorbability of water. Scanning electron microscope (SEM) images confirmed the network between laponite and PNIPAM related to their swelling behavior and crosslinking density. Small-angle X-ray scattering (SAXS) and dynamic light scattering (DLS) experiments were performed to investigate internal structure depending on the concentration and temperature.

Poster Presentation : **POLY.P-76**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Influence of surface energetics of coal graphene oxide on mechanical properties of epoxy nanocomposites

Won-Jong Choi, Soo-Jin Park[1,*]

Department of chemistry, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

Currently, carbon-based materials have been researched on their physicochemical, thermal stability, electrical and mechanical properties. Among these materials, graphene oxide (GO) has recently received considerable attention. Commonly, graphite is oxidized to GO and is then chemically or thermally reduced to produce functionalized graphite. GO is a promising candidate filler for use in composites because of its high surface area, various reaction sites, low density, high thermal resistance, and good conductivity. However, conventional GO is high-cost carbon-based material, relatively. Therefore, we fabricated coal GO and coal GO/epoxy composites in this study. Specimen of coal GO/epoxy was investigated contact angle and mechanical properties (K_{IC}, G_{IC}). We could found enhancement of surface free and mechanical properties of coal GO/epoxy composites.

Poster Presentation : **POLY.P-77**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Effects of Employing Planar Core in Quinoid-type Semiconducting Polymers

Yeonsu Choi, Yunseul Kim, Dong-Yu Kim*

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea

Lately, the quinoid-type molecules and polymers have been attracted as promising semiconducting materials for organic electronics due to their beneficial properties such as superior electrical properties, low band gap and spin characteristics. For the development of quinoid-type building blocks, the rational design of isomer-controllable core containing quinoid materials has been considered as a critical issue since the presence of geometrical isomers limits the systematic investigation of their chemicophysical properties based on structure-property relationship. In this work, a novel isomer-free and low-lying energy level isatin-terminated quinoid molecule incorporating extended aromatic rings in quinoid core was designed and synthesized by simple indophenine reaction. Then a novel conjugated polymer using the prepared quinoidal monomer was synthesized via Stille polymerization. It was found that the developed quinoidal building block exhibited the single isomer configuration, facilitated by steric hindrance between aryl rings and electrostatic intramolecular interaction between adjacent rings. Additionally, the employment of planar quinoid core had effects on the decrease of the electron-releasing mesomeric effect into conjugated backbone, resulting in significant red-shift (~ 200 nm) absorption and dramatic downshifting both HOMO (~ 0.3 eV) and LUMO (~ 0.6 eV) energy levels. The charge transport capability of the prepared quinoidal conjugated polymer was evaluated by fabricating the organic field-effect transistors, exhibiting the balanced ambipolar charge transport mobilites in both p- and n-channels.

Poster Presentation : **POLY.P-78**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Carbon dots with polymer composite transparent thin films for UV shielding and sustainable food packaging applications

Daewon Sohn*, Akshay S. Patil[1]

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The rays of sunlight are split into different spectrums, ranging from gamma rays to radio waves (high frequency to low frequency). Most of those high-frequency waves are the gamma rays, X-rays, and UV-Visible (200-400 nm) rays emitted by the sun. Maximum UV-light can be absorbed in the atmosphere, but some UV light reaches the earth's surface, which causes sunburn, skin damage, and cataract’s-like disease to occur. This study has prepared the yellow light-emitting carbon dots using amino acids and thiourea. Synthesized carbon dots and their composite with polymer for UV shielding and sustainable edible food packaging applications. These carbon dots have concentration-dependent UV absorption capacity. Carbon dots having 0.5 µL/ml absorb the until 320 nm complete 100% UV light. Optimization of the appropriate concentration of nanomaterials into a polymeric matrix to maintain physical properties like transparency, tensile (strain-stress), crystallinity, flexibility, etc. is also more significant. Along with UV shielding ability, antibacterial properties can also be imparted by the addition of chitosan-like biopolymers and antibacterial nanomaterials (Ag, ZnO, etc.) into the biopolymer matrix.

Poster Presentation : **POLY.P-79**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Bis-pyrrolidinium Ionic Polymers: Poly(methacrylate)s with Ionic Pendants and Linear Ionenes with Main-Chain Ionic Units

Jongchan Shin, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

In solid-state polymer electrolyte systems, number of mobile ions and ion dissociation behavior are important factors to enhance the ion transfer properties, which are affected by the position of ionic salt units in the polymer structure. To clarify this effect, we designed two types of ionic polymers containing C_4-bridged bis-pyrrolidinium cations: poly(methacrylate)s with the pendant bis-pyrrolidinium and linear ionenes with the main-chain same cationic units. The ionic poly(methacrylate)s were formed from the corresponding methacrylate monomers of *N*-hydroxyalkyl- *N'*-alkyl bis-pyrrolidinium PF_6^-, which were synthesized in four steps. The homopolymerizations of the ionic methacrylates were performed in surfactant-free emulsion conditions. For the linear ionenes, di(hydroxyalkyl) bis-pyrrolidinium PF_6^- monomers were used. Corresponding ionic polyesters and polyurethanes were synthesized using sebacoyl chloride or 4,4'-diphenylmethane diisocyanate, respectively and the ionic chain extender, di(hydroxyalkyl) bis-pyrrolidinium PF_6^- salts. In the presentation, detail property comparisons and characterizations will be discussed.

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Polymer Chemistry

Event Hall FRI 11:00~13:00

Investigation of open-shell quinoidal conjugated polymer for charge transport and magnetic-induced spin characteristics

Yunseul Kim, Yeonsu Choi, Dong-Yu Kim[*]

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Open-shell conjugated polymers have radicals (unpaired electrons) in polymers, which demonstrate narrow band-gap, multiple oxidation/ reduction states and unique spin characteristics as well as spin-induced magnetic properties. They have shown considerable promise for next-generation flexible electronics such as organic photovoltaics (OPVs), organic field-effect transistors (OFETs), organic thermoelectrics and organic spintronics. Quinoid structure is linked by double bond between each ring, and it can stabilize the open-shell form with diradical upon recovery of aromaticity. Thus, the introduction of the open-shell type quinoidal building blocks into polymer backbone is an effective strategy for development of an open-shell conjugated polymer with high spin characteristics. In this research, we will present our recent results on the investigation of structure-property relationship of an open-shell conjugated polymer embedded with diradicals. We designed and synthesized an azaisatin-terminated quinoid building block, azaquinoidal-bithiophene (azaQuBT), which has pyridine replacing benzene in the end of terminal isatin unit. This can lead to better coplanar conformation of polymer backbone due to reducing the torsional angle between quinoid and comonomer counterpart. Therefore, diradicals, which is occurred by open-shell form of azaQuBT, could be well-delocalized into the polymer backbone, leading to stable high-spin ground-state. An open-shell conjugated polymers, PazaQuBT-T, was successfully synthesized via Stille-polymerization. We calculated the diradical character and singlet-triplet energy difference and characterized optical, electronic, and spin-induced magnetic properties through UV-Vis-NIR absorption, Raman spectroscopy, electron spin resonance (ESR), magnetic property measurement system (MPMS) and discussed.

Poster Presentation : **POLY.P-81**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Characterization of Pyrrolidinium-Jeffamine® Co-poly(amide-ester)s

Choi Jong in, Minjae Lee[1,*], Jongchan Shin[2]

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[2]*Kunsan National University, Korea*

A new series of ionic co-poly(amide-esters)s containing pyrrolidinium salt units were synthesized from di(hydroxyalkyl) pyrrolidinium salt (0.5 equiv.), Jeffamine ed2003 (0.5 equiv.) and sebacoyl chloride (or terephthaloyl chloride) (1.0 equiv.). FT-IR analysis gave the reaction completion when the 1780 cm^{-1} carbonyl peak (acyl chloride) totally disappeared, and 1715 cm^{-1} (ester) and 1650 cm^{-1} (amide) peaks appeared. ^1H NMR analyses showed the exact mole ratio between the ionic and the non-ionic monomer ratio in the synthesized copolymers. The thermal stability of all the synthesized ionene co-poly(amide-ester)s was investigated by thermogravimetric analysis (TGA) and were stable up to 220 °C. Differential scanning calorimetry (DSC) analysis showed semi-crystalline phase(s) below their melting point (T_m). The melting transition was due to crystallization of the PEG segments in Jeffamine ed2003. Detail thermal properties and ionic conductivities of the copolymers and their composites with Li salt will be discussed in the presentation.

Poster Presentation : **POLY.P-82**

Polymer Chemistry

Event Hall FRI 11:00~13:00

CpG Incorporated DNA Micelle for Immunological Treatment of HIV-1

Hae Joo Kim, Jun-O Jin[1], Peter Chang Whan Lee[2], Minseok Kwak[3,*]

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[3]*Department of Industry 4.0 Convergence Bionics Engineering and Department of Chemistry, Pukyong National University, Korea*

Unmethylated CpG motifs activate toll-like receptor 9 (TLR9), leading to sequence- and species-specific immune stimulation. Here, we engineered a CpG oligodeoxyribonucleotide (ODN) with multiple hydrophobic moieties, so-called lipid-modified uracil, which resulted in a facile micelle formation of the stimulant. The self-assembled CpG nanostructure (U4CpG) containing the ODN 2216 sequence was characterized by various spectroscopic and microscopic methods together with molecular dynamics simulations. Next, we evaluated the nano-immunostimulant for enhancement of anti-HIV immunity. U4CpG treatment induced activation of plasmacytoid dendritic cells (pDCs) and natural killer (NK) cells in healthy human peripheral blood, which produced type I interferons (IFNs) and IFN-γ in human peripheral blood mononuclear cells (PBMCs). Moreover, we validated the activation and promotion efficacy of U4CpG in patient-derived blood cells, and HIV-1 spread was significantly suppressed by a low dosage of the immunostimulant. Furthermore, U4CpG-treated PBMC cultured medium elicited transcription of latent HIV-1 in U1 cells indicating that U4CpG reversed HIV-1 latency. Thus, the functions of U4CpG in eradicating HIV-1 by enhancing immunity and reversing latency make the material a potential candidate for clinical studies dealing with viral infection.

Poster Presentation : **POLY.P-83**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Polymeric nanoparticles loaded Lumogen® dyes for cellular detection and imaging

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Lumogen fluorescent dyes have great light stability as well as high fluorescence quantum yields. Despite of the excellent photophysical properties of dyes, the highly hydrophobic structure in common makes the compounds difficult to function as biological fluorescence probes. To generally utilize a family of organic fluorescent dyes such as Lumogen® Red, Orange, Yellow, and Violet, as a biomarker for cellular imaging in flow cytometry and fluorescence microscopy, we used an encapsulation method using amphiphilic block copolymer namely Pluronic® F127. Cell uptake of the probe nanoparticles by HeLa cells was analyzed by flow cytometry and confocal laser scanning microscopy.

Poster Presentation : **POLY.P-84**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Scission of a specific covalent bond by mechanical force transferred through DNA

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An ultrasound-induced bond cleavage on mechanopore (MP), which is a weak bond along the polymer chains, is one of the main fields of polymer mechanical chemistry. To date, there are not many studies on the role of polymers, which are mechanical force carriers. Here we report precisely prepared DNAs as the mechanocarriers (MCs) instead of conventional polymers for the mechanochemical bond scission. For this study, a DNA-MP-DNA structure was designed in which an MP is located at the center and two DNA MCs are connected to both termini. We mainly used polymerase chain reaction to engineer DNA MCs and ultrasound as the mechanical force. The effect of DNA MCs was evaluated by changing the length, rigidity, and shape of DNA segments. We investigated to precisely control the bond scission by external force transmitted to MPs through DNA MCs.

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Poster Presentation : **POLY.P-85**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Device for real-time non-contact infrared thermal measurement and processing

Hyosung Choi, Banyu Firdaus Soeriawidjaja, Sang Hak Lee[1], Minseok Kwak[2,*]

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Temperature is one of crucial and integral parts of chemical experiments. Since the properties or shape of the material may change depending on the temperature, the device that measures it plays a vital role in an experiment. Such devices commonly used in experiments to this day are unable to perform temperature measurement and data processing simultaneously. Here, we present a low-price, non-contact convenient platform capable of solving both problems at the same time, with automatically set different measurement time intervals for each experiment, and shows processed data anywhere real-time on the Internet. This device can operate within temperature range of -20°C and 80°C with a respectable error range of ±2.5°C.

Poster Presentation : **POLY.P-86**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Preparation of lactic acid-based plasticizer for improving flexibility of transparent poly(lactic acid)

Hyemin Yang, Jeyoung Park[*]

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Poly(lactic acid) (PLA), the most popular biodegradable plastic, has high mechanical properties, excellent transparency, and processability. Despite these advantages of PLA, its inherent brittleness and poor thermal stability restrict its wide application. In order to improve brittleness, a new plasticizer is added in the industrial fields, which however loses its transparency.To overcome its drawbacks, PLA was blended with a novel PLA oligomer by direct condensation at various compositions, and their compatibility, optical properties, and crystallization behavior were examined by 1H-NMR, scanning electron microscopy (SEM), differential scanning calorimetry (DSC), and tensile testing. Especially, the plasticizer makes PLA increase elongation up to 50 times higher while maintaining transparency.

Poster Presentation : **POLY.P-87**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Highly-photostable polymeric nanoparticles for encapsulating near-infrared dye under hyperthermal irradiation.

Banyu firdaus Soeriawidjaja, Mingyeong Kang, Minseok Kwak[1,*]

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Polymeric micelles are suitable nanocarriers to load hydrophobic molecules within the core in aqueous media. We report nanoparticles that the polymeric micelles encapsulate organic near-infrared (NIR) dye, IR788, as a photoabsorbing agent for generating heat under NIR irradiation. In addition, the core of micelle is structurally stabilized via semi-interpenetrating network formation, which represents enhanced photostability, more stable loading environment under low temperature and enhances biocompatibility in cell experiment compared to indocyanine green.

Poster Presentation : **POLY.P-88**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Ca-based Paramagnetic Nanoparticle Catalyst for Chemical Recycling of PET

Jeongwook Hwang, Yonghwan Kim*

Advanced Materials R&D Center, DAE-IL Corporation, Korea

In this study, Polyethylene terephthalate (PET) waste was depolymerized into bis(2-hydroxyethyl)terephthalate (BHET) through glycolysis with the Ca-based paramagnetic nanoparticle catalyst. Especially, the effect of heat treatment on the catalyst prepared by the co-precipitation methods was investigated through XRD (x-ray diffraction), SEM (scanning electron microscopy), VSM (vibrating sample magnetometer) to enhance the catalytic effect. As the temperature of heat treatment increased, the phases of core-shell boundary of the catalyst were converted from $Ca(OH)_2$ to $Ca_2Fe_2O_5$ and CaO. At the same time, the phase fraction of $Ca_2Fe_2O_5$ increased, and the phase fraction of Fe_3O_4 decreased. The highest fraction of Fe_3O_4 was obtained at 350°C, which is a relatively low temperature, and the saturation magnetic force of the catalyst was 47.16 emu/g. As a result of glycolysis process, the maximum BHET yield was 88.84% under the reaction conditions of mass ratios (EG to PET = 5, catalyst to PET = 0.1) at 196℃ for 3h. In particular, the repeated experiments were performed to verify the stability of catalyst reusability, and the magnetic particle catalyst was recycled for 10 times.

Poster Presentation : **POLY.P-89**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Influence of Material Properties on the Damage-Reporting and Self-Healing Performance of a Mechanically Active Dynamic Network Polymer in Coating Applications

Mi Ju Bae, Jin Chul Kim[*], Young Il Park[1,*], In Woo Cheong[2,*], Ja-Hyoung Ryu[3,*]

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Herein, we investigated about the influence of dynamic polymer network coatings on their self-healing and damage-reporting performance. A series of reversible polyacrylate urethane networks containing the damage-reporting diarylbibenzofuranone unit were synthesized, and their material properties (e.g., indentation modulus, hardness modulus, and glass-transition temperature) were measured conducting nanoindentation and differential scanning calorimetry experiments. In the soft polymer network and hard polymer network-combined coating, the damage-reporting and self-healing performances of the dynamic polymer network coatings exhibited opposite tendencies with respect to the material properties of the polymer network coatings. These features of the dynamic polymer network coatings are unique; they are not observed in elastomers, films, and hydrogels, whereby the polymer networks are bound to the substrate surface. Evidence indicates that controlling the polymer's physical properties is a key factor in designing high-performance self-healing and damage-reporting polymer coatings based on mechanophores

Poster Presentation : **POLY.P-90**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Synergetic Effect of an Additive in One-pot Mechanosynthesis of Polymer-CNT Composites

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Dispersing carbon nanotubes (CNT) into polymer matrix against its aggregation nature is generally required using toxic solvents, massive amount of energy and times. Here we demonstrate a time efficient and eco-friendly fabrication of dynamically crosslinked polymers and polymer-CNT composites via additive assisted mehchanosynthesis without solvent. Carefully chosen additive prevents thermal oxidation of polymer chains, enhances polymers mechanical properties and recylability without disturbing CNT dispersity in composites.

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Poster Presentation : **POLY.P-91**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Cyclohexyl-substituted Non-fullerene Acceptors for Organic Solar Cells

Chanbeom Park, Guseon Kim, Eunhee Lim*

Department of Applied Chemistry, University of Seoul, Korea

As a result of much interest and research on organic solar cells (OSCs) over the past decade, the power conversion efficiencies (PCEs) of OSCs reach 18%. OSCs have various advantages such as ease of process, flexibility, low cost, lightness, and transparency. It is believed that OSCs can be commercialized if problems such as cost, durability, large-area fabrication, and eco-friendly process are solved. In this study, two non-fullerene acceptors (NFAs) with a simple molecular structure were easily synthesized. Two cyclohexyl-substituted non-fullerene small molecules are designed to have the same molecular backbone of a bithiophene core and rhodanine end groups. The optical, thermal, and electrochemical properties of the NFAs were investigated, and a PCE of 6.91% was obtained under additive- and annealing-free conditions. Such a simple manufacturing process can satisfy one of the prerequisites for OSC commercializatio

Poster Presentation : **POLY.P-92**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Siloxane-Terminated Side Chain Engineering on Dithienobenzothiadiazole-Based Wide Band Gap Polymer donor in Non-Fullerene Polymer Solar Cells

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In this work, a wide band gap (WBG) polymer donor based on dithienobenzothiadiazole (DTBT) and benzodithiophene (BDT) was explored for the organic solar cells. Siloxane based side chain was introduced on BDT unit to further improve the solubility, blend miscibility and film morphology. New polymer DT-Sil-B was synthesized and systematically carried out the characterizations. DT-Sil-B showed film absorption peak at 450 nm and optical band gap of 2.19 eV. The complementary absorption and energy offsets observed between DT-Sil-B polymer donor and IT-4F acceptor. The DT-Sil-B:IT-4F based OSCs resulted an open-circuit voltage of 0.78 V, a short-circuit current density of 16.60 mA cm−2, and a fill factor of 62.56%, corresponding to a power conversion efficiency (PCE) of 8.15%. Further optimizations can enhance the performance of DT-Sil-B based OSCs. The results emphasize that DT-Sil-B can be a powerful donor, which is favorable in the construction of simple WBG polymer donors for efficient NFA based PSCs.

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Poster Presentation : **POLY.P-93**
Polymer Chemistry
Event Hall FRI 11:00~13:00

Impact of Rhodanine End-groups on Benzotriazole based Non-fullerene Acceptors

Jeonghyeon Kim, Jieun Lee, Priyanka Yadav[1], Sung-Ho Jin[2,*]

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Non-fullerene acceptor (NFA) materials with low optical bandgap (Egopt) are essential for developing efficient and stable organic solar cells (OSCs) with high power conversion efficiencies (PCEs). Herein, we synthesized a new NFA namely, (5E,5'E)-5,5'-((12,13-bis(2-ethylhexyl)-6-hexyl-3,9-diundecyl-12,13-dihydro-6H-thieno[2'',3'':4',5']thieno[2',3':4,5]pyrrolo[3,2-g]thieno[2',3':4,5]thieno[3,2-b][1,2,3]triazolo[4,5-e]indole-2,10-diyl)bis(methanylylidene))bis(3-ethyl-2-thioxothiazolidin-4-one) (BTUDR). The thermal, photophysical and electrochemical properties were systematically investigated. Interestingly, BTUDR exhibited low Egopt of 1.83 eV with suitable frontier molecular orbital (FMO) energy levels, highest occupied molecular orbital (HOMO) = -5.59 eV and lowest unoccupied molecular orbital (LUMO) = -3.76 eV. BTUDR was thermally stable up to 330 ˚C as revealed by its thermogravimetric analysis (TGA) (5% weight loss). The differential scanning calorimetry (DSC) results indicated that the melting (Tm) and crystallization (Tc) temperatures of BTUDR were 78℃ and 166℃ respectively. Therefore, BTUDR blended with polymer PM6 exhibited a PCE of 9.70%, open-circuit voltage (Voc) of 0.85V, a short-circuit current density (Jsc) of 21.19 mA/cm2, and fill factor (FF) of 54.34%, respectively.

Poster Presentation : **POLY.P-94**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Achieving over 20% Efficiency in Perovskite Solar Cells with Dopant-Free Polymeric Hole Transport Material by Side Chain Strategy

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At present, spiro-OMeTAD is the most widely used HTM in the n-i-p type PSCs.[1-2] However, the spiro-OMeTAD shows low hole mobility and electrical conductivity in their original forms, which affect device performances.[3] Consequently, the p-type dopants, such as Li-TFSI and tBP, were used as additives to improve their charge transport performance.[4] However, the dopants in HTMs can hygroscopic and accelerate the decomposition of the perovskite layer, which can lead to the poor stability of the PSCs device and block commercialization. Therefore, the exploration of doped-free, high-efficiency HTMs has always been the direction of our efforts. Here, a new polymer electron-donor material, Nap-SiBTz3, is designed and synthesized as a dopant-free HTM in PSCs. A champion PCE of 20.79% with a Jsc of 25.01 mA/cm2, Voc of 1.10 V and FF of 75.81% was achieved. Besides, the devices show long-term stability and these studies give useful guidance on exploiting efficient dopant-free HTMs of PSCs.

Poster Presentation : **POLY.P-95**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Investigation of Monodiperse Metal Labelled Polystyrene Particles as Internal Standard for Mass Cytometry

Yoolee Lee, Daewon Sohn[1,*]

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A technique called mass cytometry allows 40 cells to be separated simultaneously at a time, which requires each cell to have a lanthanide marker. Since labelled cells are nebulized and flow to argon plasma, which ionizes the metal-labelled antibodies. Then the metal signals are analyzed by a TOF (time-of-flight) mass spectrometer. For cell counting, internal standards are necessary. The particles should be suitable for mass cytometry calibration as internal standards. To perform these roles, metal-labelled microspheres were required to have monodispersity, functionality and metal content criteria. The material of the bead particle is selected as polystyrene, which can be applied in many ways, and is easily synthesized, stable, and can be made into various forms as well as applying various functional group to the surface, making it suitable for cytometry's standardization bead. In this study, polystyrene based smaller particles with quantified concentration has been studied for further application in bioanalysis. Polystyrene particle containing lanthanide metal such as Eu is fabricated by nanoprecipitation polymerization for making more monodisperse particles. The size and the morphology of the synthesized beads have been characterized by dynamic light scattering (DLS), scanning electron microscope (SEM), and Eu content of each particle has been determined by single-particle inductively coupled plasma mass spectrometer (spICP-MS).

Poster Presentation : **POLY.P-96**

Polymer Chemistry

Event Hall FRI 11:00~13:00

Advantages in gas adsorption of adsorbents synthesized with modified halloysite nanotubes and metal-organic frameworks.

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Halloysite nanotubes, MOF were used as gas adsorbents. It was judged that the complex of halloysite and MOF could significantly increase the gas adsorption capacity, so the synthesis of HNTs, MOF complex was conducted focusing on nitrogen and carbon dioxide adsorption experiments.Gas adsorbents were synthesized with the modified HNTs and MOFs, HKUST-1, the most widely studied MOFs owing to their high porosity. And HNTs were used for surface modification after only purifying. Hybrid composites synthesized by the solvothermal method by loading the MOF precursor into the lumen of the surface-modified HNTs are referred to as EHNT@HKUST-1 and HNT-NH_2@HKUST-1.The gas adsorption capacity was analyzed by Brunauer-Emmett-Teller (BET) using N_2 and CO_2 gases. Specifically, the EHNT@HKUST-1 composite showed enhanced CO_2 gas adsorption capacity compared to HNT@HKSUT-1, being increased about 14.9 times, from 8.344 cm^3(STP)g-1 to 19.332 cm^3(STP)g-1. Additionally, HNT-NH_2@HKUST-1 indicated around 24.849 cm^3(STP)g-1 of CO_2 gas adsorption capacity. Additionally the morphological and structural characteristics were also analyzed by SEM, TEM-EDS, and XRD. Looking at the images, it can be seen that the MOF grows along the inner wall of the tube to match the shape of the longitudinal axis, which is noteworthy data. It is also speculated that by inserting the MOF inside the tube, the moisture vulnerability of the MOF itself could be supplemented.

Poster Presentation : **IND.P-1**
Industrial Chemistry
Event Hall THU 11:00~13:00

Ultrasensitive Chiral Recognition of Enantiomers using Plasmonic Chirality Enhancer

Juyong Gwak, Jaebeom Lee[1,*]

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The recognition and separation of enantiomeric molecules, oligomers, and polymers have been challenging for efficient chiral sensing and drug safety in pharmaceutical and biomedical industries. Recently, we have introduced a novel approach to monitor chiral moieties via helical magnetic field (hB) where chiral-active magnetoplasmonic nanoparticles (MagPlas NPs) were assembled into helical nanochain structure. In the article, the feasibility of the hB-induced chiral sensing has been demonstrated. Ag@Fe3O4 core-shell NPs were used for magnetic field-responsive plasmonic nanomaterials while an in-house hB generator, aka., plasmonic chirality enhancer was fabricated. Helically-aligned MagPlas NPs in the enhancer showed remarkable circular dichroism (CD) properties that can correlate with other chiral analytes, leading to enhancing the CD signals at the lower concentration than the technical limit of detection (LOD), i.e., 10-7 M of the commercial CD spectrometry, finally reaching to 10-10 M. The computation simulation announced that the total chiroptical properties of MagPlas NP chains under hB were readily changed by modifying chiral structure of analytes, the interchain distance of MagPlas NP, and configuration of alignment. When the right or left circularly polarized (RCP/LCP) light interacted with the chiral molecule, a unique fluctuation of the circularly irradiated light was observed compared with the same nanochain system without the chiral molecule. This hB-induced chirality enhancer presents an advanced tool to recognize chiral materials qualitatively and quantitatively, enabling further practical applications in chiroptical recognition in pharmaceutical and biomedical sensing and imaging.

Poster Presentation : **IND.P-2**
Industrial Chemistry
Event Hall THU 11:00~13:00

Production of Gaseous Chlorine Dioxide for the Disinfection of Livestock-related Facilities including Personnels and Automobiles to prevent Livestock Diseases.

Jung Hyuck Cho

R/D Center, NEOCL (LLC), Korea

A new and low-cost preparation method of chlorine dioxide for the disinfection of livestock-related facilities including personnels and automobiles was developed. Recently, livestock diseases are on the rise, and various viruses and bacteria have been pointed out as the cause, so their elimination is an important issue in the livestock industry. Chlorine dioxide was chosen as the first priority disinfectant for the removal of variousmicroorganism including bacteria,virus and protozoa as well as for the removal of malodor in the livestock-related facilities. But its inherent self-decomposition property limited in its broad spectrum use . In addition, since chlorine dioxide uses expensive sodium chlorite as a main raw material in its manufacture, an economical manufacturing method is very necessary. Sodium chlorate is oxidized under acidic conditions to generate chlorine dioxide. Sodium chlorate is 1/3 the price compared to sodium chlorite, and the chlorine dioxide generation yield is high. The reaction proceeds at a relatively high temperature of 60 degrees Celsius, and chlorine dioxide gas generated by bubbling air into the generator is injected into the livestock-related facilities through a duct. Personnel and vehicles entering and exiting the livestock-related facilities are also sterilized with gaseous chlorine dioxide, which protects the facilities from various bacteria and viruses to prevent livestock diseases.

Poster Presentation : **IND.P-3**

Industrial Chemistry

Event Hall THU 11:00~13:00

Usage of Radioisotope at Industrial institute

Bo Bae Cho[*], **Suengil Park**[1]

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Usage of Radioiosotopes for diverse industrials application was increasing. Especally, medical application interest such as diagnosis and treatment is higher and It cause need of much local production of radioisotopes. Radioisotopes are generally produced by Cyclotron and reactor. But the most of radioisotopes in Korea was obtained from abroad because Reactor was stopped the operation and Cyclotron for production was rare and the many radioisotopes production method was not developed. From now on, the effort for diverse radioisotopes production and the information of radioisotopes which is need for urgent research or usage are very important. In this research, we investigate which radioisotope was using for which usage and how getting it at many industrial Institute. furthermore, the species of radioisotopes need in future was investigated.

Poster Presentation : **IND.P-4**
Industrial Chemistry
Event Hall THU 11:00~13:00

Efficient Blue Phosphorescence from Homoleptic Cyclometalated Dibenzothiophene/Dibenzofuran–NHC–Iridium(III) Complexes

Bo-Sun Yun, Min Su Choe, Daehan Lee, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

The NHC–Ir complexes f-IrS_{iPr}, m-IrS_{iPr}, and m-IrS_{Me}, in which a dibenzothiophene (DBT) moiety is used to increase the emission efficiency for deep-blue phosphorescence, were synthesized and compared with the dibenzofuran (DBF)-based Ir complexes f-IrO_{Me} and m-IrO_{Me}. The differences in the ligand structure (DBF/DBT) or configuration (fac/mer) of these complexes led to different electrochemical and photophysical properties. The DBF moiety has a stronger electronegativity than DBT, resulting in a larger T_1–S_0 energy gap and a shorter emission wavelength than those of the DBT complexes. On the other hand, the meridional isomer has a mutually trans-phenyl ligand configuration that leads to lengthening of the transoid Ir–C bond and destabilizes the HOMO level, resulting in greater ease of oxidation, and the emission is red-shifted relative to the facial forms. Even with the differences in the origin of phosphorescence, replacement of the oxygen atom in the DBF unit with sulfur does not greatly alter the emission efficiency in either solution or film while achieving the same high-end deep-blue phosphorescence with unprecedented CIE coordinates of [0.14, 0.19] for m-IrS_{Me} (EQEmax; 17.1%) and [0.14, 0.14] for m-IrO_{Me} (EQEmax; 18.2%).

Poster Presentation : **IND.P-5**
Industrial Chemistry
Event Hall THU 11:00~13:00

Photophysical Properties of Homoleptic Ir(III) Complexes Bearing Bulky Aryl-Substituted N-Heterocyclic Carbene (NHC) Ligands

Bo-Sun Yun, Sunghan Choi, Daehan Lee, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

The phosphorescence properties of fac-Ir(pmp)3, mer-Ir(pmp)3, fac-Ir(dmpmp)3 and mer-Ir(dmpmp)3 (where pmp = 3-methyl-1-phenyl-2,3-dihydro-1H-imidazo[4,5-b]pyridine and dmpmp = 1-(20 ,60 -dimethylbiphenyl-2- yl)-3-methyl-2,3-dihydro-1H-imidazo[4,5-b]pyridine) in CH2Cl2 were investigated. At 77 K, the fac-isomers showed blue emission with a vibronic structure, while the mer-isomers showed less structured emissions. At 300 K, all complexes showed broad and markedly red-shifted emission spectra compared to those at 77 K. The quantum yields of the Ir(dmpmp)3 isomers were very low, and their emission lifetimes were very short compared to those of Ir(pmp)3. In order to understand the large differences between the photodynamic properties of Ir(pmp)3 and Ir(dmpmp)3, we performed femtosecond time-resolved transient absorption (TA) spectroscopic measurements. The TA spectra of Ir(dmpmp)3 were almost the same as those of Ir(pmp)3 at a short delay time. However, Ir(dmpmp)3 showed a new broad TA band at around 720 nm with increasing delay time. The rise time of this band was ca. 10 ps for both isomers, and this may be attributed to the geometrical change in the excited state, which is associated with the steric hindrance of the bulky dimethylphenyl substituent. Actually, Ir(dmpmp)3 showed a strong rigidochromic shift in the emission spectra with varying temperature. To understand the molecular orbitals and the energy levels, theoretical calculations were performed using density functional theory. As a result, structural displacement takes place accompanied by the fast migration of localization of excited states via intraligand charge transfer

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Poster Presentation : **IND.P-6**
Industrial Chemistry
Event Hall THU 11:00~13:00

Excited-State Modulation of Blue Phosphorescent Ir(III) Complex via Alteration of the Heterocyclic Group of Chelating Carbene Ligand

Bo-Sun Yun, Min Su Choe, Sunghan Choi, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A series of Ir(III) complexes (fac-Ir(py), fac-Ir(pz), fac-/mer-Ir(im), and fac-/mer-Ir(bzim)) with 9,9-dimethylfluorenyl (dmf)-based ligands (dmfC^N or dmfC^C:) tuned with various heterocyclic chelating moieties (pyridyl (py), pyrazolyl (pz), imidazolyl (im), and benzimidazolyl (bzim)) were prepared and investigated for the development of novel efficient blue phosphorescent dopants. Of these Ir(III) complexes, mer-Ir(im) complex was compared with the previously reported Ir(III) complexes, i.e., mer-tris(N-phenyl-N'-methylimidazole)iridium (mer-Ir(pim)), mer-tris(N-dibenzofuranylphenyl-N'-methylimidazole)iridium (mer-Ir(im-O)), and mer-tris(N-dibenzothiophenyl-N'-methylimidazole)iridium (mer-Ir(im-S)), and the effect of replacing the phenyl group of the phenylimidazole ligand with a dmf moiety was also investigated. Steady-state photophysical analysis confirmed that the observed emission colors were tunable from λem = 545 nm (fac-Ir(py)) to λem = 462 nm (fac-Ir(bzim)) depending on the heterocycle type. In addition, the lower absorption and emission energies were observed when the phenyl moiety was extended to the dmf analogues of the phenylimidazole ligand. From DFT/TD-DFT calculations and electrochemical analysis, we found that the relative degree of MLCT contribution in 3MLCT/3LC admixture-based emission process and the structural distortion (ΔQe) between the excited and ground states affect the quantum efficiencies and radiative rate constants of the Ir(III) complexes, which is related to the electroluminescence performance. The mer-Ir(im) and fac-/mer-Ir(bzim) with high emission quantum yields of ≥85% in the film state were evaluated as dopant materials in blue PhOLEDs.

Poster Presentation : **IND.P-7**
Industrial Chemistry
Event Hall THU 11:00~13:00

Home-built solid-state NMR probes for the analysis of specific materials

Minseon Kim, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Solid-state NMR is used to investigate insoluble substances such as various organic/inorganic nanomaterials, biosolids, polymers, pharmaceuticals, membrane proteins. Depending on the variety of materials, selecting the appropriate probe for the purpose is an important step in achieving the desired results. We strive to create specific probes that are highly efficient and durable for various samples. Here, we present the coil design, construction, efficiency, and optimized design of home-built 400 MHz narrow-bore (NB) and wide bore (WB) 1H-15N solid-state NMR probes and a home-built 800 MHz NB 1H-15N solid-state NMR probe for lossy samples. A 400 MHz and 500 MHz NB 19F-13C solid-state NMR probe for analyzing nanomaterial and 600 MHz NB 19F-7Li solid-state NMR probe with solenoid coils for investigating Li-ion battery were developed and manufactured. In addition, 400 MHz NB 1H-31P double-resonance solid-state NMR probe with scroll coil was designed and constructed for the analysis of biological samples containing phosphorus and various materials. For all home-built probes, preliminary NMR data were acquired to demonstrate their effectiveness.

Poster Presentation : **IND.P-8**
Industrial Chemistry
Event Hall THU 11:00~13:00

Development of Low-formaldehyde amino resin by removing hexamethylenetetramine urotropine

Gyo Eun Gu, Jong Hwi Park[1,*]

Development of PU materials, Aekyung Chemical Co., Korea
[1]*PU Materials Development, aekyungchemical, Korea*

There are many types of curing agents used in the market today. Among them, amino resin is obtained by a condensation reaction between formaldehyde and amino compounds contained amine(NH2) groups. Amino-formaldehyde resins can be used with acrylic, alkyd, polyester and epoxy resins to produce superior coating properties. However, due to safety issues of formaldehyde, the application of amino resin is limited by strict regulations in each country despite the excellent strength of the resin. Accordingly, in the industry, many studies are being conducted to remove residual formaldehyde from the amino-formaldehyde resin. In this study, a low-formaldehyde(LF) resin have been prepared by reacting formaldehyde and ammonia solution(NH4OH) under xylene to produce hexamethylenetetramine urotropin, an aqueous precipitate. This precipitate has been removed through evaperation and filteration process. Consequently, the formaldehyde content of the resin can be reduced by 3.39% from 5.08% to 1.69%.

Poster Presentation : **IND.P-9**

Industrial Chemistry

Event Hall THU 11:00~13:00

Artemisinin is a good lead natural compound for developing antiviral agents that can control RNA viruses

Seok Joon Lee[*], **Sangtae Oh**[1]

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[1]*Department of Basic Sciences, College of Medicine, Catholic Kwandong University, Korea*

Recently, considering the situation such as the Covid pandemic, it is very important and urgent to develop various antiviral drugs in order to prepare for the coming risks in advance. We screened various natural products or their derivatives to see if they could be used as drugs capable of inhibiting RNA viruses. Among them, artemisinin was found to be a compound suitable for that purpose. The natural sesquiterpene endoperoxide artemisinin, which was isolated from Artemisia annua L., has become a useful lead compound in the development of antimalarial drugs. Its applicability is also expanding into the fields of tumor, viral, fungal infection, and unwanted immune response in transplantation. In this presentation, we will show an example in which artemisinin derivatives can be developed as antiviral agents that can control various RNA viruses.

Poster Presentation : **IND.P-10**

Industrial Chemistry

Event Hall THU 11:00~13:00

Development of high-water dispersible polyisocyanate by introducing ionic or unionic reacting surfactant

Hye Lin Choi, Kyung Jin Kim*

PU Materials Development, Aekyung Chemical, Korea

Polyisocyanate curing agents can be used with polyols in urethane paint. Urethane paint usually consist of polyols, polyisocyanate curing agents, pigments, additives and solvents. Among the components, organic solvents are usually used, which may volatilize into the atmosphere and cause air pollution. Recently, as environmental regulations are strengthened, urethane paint needs to be changed. Therefore, in this study, the purpose is to develop a polyisocyanate curing agent that can be used by replacing the organic solvent with water. It is obtained using reactive ionic emulsifiers or non-ionic emulsifiers and we can implement particle size of 150 nm or less by diluting a curing agent in water.

Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Zn(II) Metal-Organic Frameworks with Different Dimensionality Controlled by Solvothermal Reactions

Jihye Oh, Dong Hee Lee, In-Hyeok Park*

Graduate School of Analytical Science and Technology, Chungnam National University, Korea

We report two metal-organic frameworks (MOFs) with dimensionality controlled by different reaction conditions. The two- and three-dimensional Zn(II) MOFs (**1** and **2**) derived from an olefinic dipyridyl ligand 1,4-bis[2-(4'-pyridyl)ethenyl]benzene (bpeb) and 1,3-benzenedicarboxylic acid (m-H_2bdc) were prepared. The yellowish single crystals of two-dimensional MOF, $[Zn_2(m\text{-bdc})_2(\text{bpeb})_2]\cdot 2DMA$ (**1**) and three-dimensional MOF, $[Zn_3(m\text{-bdc})_3(\text{bpeb})_2(H_2O)_{0.5}]\cdot H_2O$ (**2**) were obtained under solvothermal reaction with a mixture of different solvent conditions. The coordination environment of dizinc(II) cluster unit of **1** was coordinated by two nitrogen atoms of bpeb ligands and four oxygen atoms of *m*-bdc ligands. On the other hand, the trinuclear repeating unit of **2** consists of three Zn(II) atoms, two bpeb ligands, three *m*-bdc ligands and a half of a water molecule. According to Schmidt's Criteria,[1] when the distance between the C=C bond of adjacent olefin is 3.6 to 4.1 Å, olefins can be showing photoreactivity. The distance between the olefin of **1** and **2** obtained through single crystal X-ray diffractometer are 3.8 Å and 3.5 Å, respectively. Thus, both MOFs are expected to have photoreactivity. The details will be presented at the poster section.

Reference

[1] G. M. J. Schmidt, Photodimerization in the solid state, *Pure Appl. Chem.*, **1971**, *27*, 647-678.

Poster Presentation : **INOR.P-98**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

A Zigzag One-Dimensional Metal-Organic Framework incorporating Two Ligands Disordered and Its Photo-Cycloaddition Reaction

Soyun Kim, Dong Hee Lee, In-Hyeok Park*

Graduate School of Analytical Science and Technology, Chungnam National University, Korea

Metal-Organic Frameworks (MOFs) is defined as porous coordination polymers which are composed of metal ions and organic ligands.[1-3] When organic ligands of similar size are used, the different organic molecules can exist in the same space at the same time between metal cations. Here we report a zinc-based one-dimensional (1D) zigzag metal-organic framework incorporating similar lengths of *trans*-2-(4-phridyl)-4-vinyl benzoic acid (Hpvba) and 4,4’-biphenyldicarboxylic acid (H_2bpdc) disordered. A double-stranded 1D MOF, [Zn(pvba)(bpdc)(H_2O)$_2$] (**1**) is purple plate-shaped crystals, which is obtained under a mixture of dimethylformamide (DMF) and H_2O condition through solvothermal reaction of $Zn(NO_3)_2·6H_2O$, Hpvba, and H_2bpdc. The dinuclear repeating unit consists of two Zn(II) atoms, one pvba ligand, one bpdc ligand and four H_2O molecules. Zn1 in MOF **1** is tertrahedrally coordinated by one nitrogen atom of one pvba ligand and one oxygen atom of one bpdc ligand and two oxygen atoms of H_2O. In this case, these two ligands have similar lengths, so it was disordered at a 1:1 ratio, which was confirmed by ^{1}H nuclear magnetic resonance (NMR) analysis. If adjacent ligands exist simultaneously as a pvba ligand containing C=C, there is a possibility of the cycloaddition reaction under UV light. The distance between pvba ligands are 4.2 Å which meet Schmidt's Criteria (3.6-4.1 Å).[4] After UV irradiation of **1** for 48h, the formation of cyclobutane peaks were observed and checked by NMR. The details will be presented at the poster section.

References

[1] L. R. Macgillivray *et al.*, *Acc. Chem. Res.*, **2008**, *41*, 280.

[2] J. J. Vittal *et al.*, *Angew. Chem. Int. Ed.*, **2005**, *44*, 2237.

[3] J. J. Vittal *et al., Chem. Commun.,* **2008**, 5277.

[4] G. M. J. Schmidt, *Pure Appl. Chem.,* **1971**, *27*, 647-678.

Poster Presentation : **INOR.P-99**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Solvent Mediated Photoreactivity of One-Dimensional Zn(II) Metal-Organic Frameworks

Dong Hee Lee, In-Hyeok Park*

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Photoreactivity in the MOFs has a great impact on solid state chemistry.[1] In this work, we identify the significant correlation of solvents and coordination environments. Through solvothermal reaction of $Zn(NO_3)_2\cdot6H_2O$, 1,4-bis[2-(4'-pyridyl)ethenyl]benzene (bpeb), and 1-adamantanecarboxylic acid (Hadc), two types of Zn(II) based MOFs are prepared under different solvent conditions. A 1D railroad MOF, $[Zn_2(bpeb)_2(adc)_4]$ (**1**) is synthesized from dimethylacetamide (DMA) which is yellow block-shaped crystals. The dinuclear repeating unit consists of two Zn(II), two bpeb ligands and four adc ligands. Zn atoms are hexagonally six-coordinated by two nitrogen atoms of bpeb ligands and four oxygen atoms of adc ligands. On the other hand, a 1D railroad MOF, $[Zn_2(bpeb)_2(adc)_3(fa)]$ (**2**) is synthesized from dimethylformamide (DMF) which is colorless yellow block-shaped crystals. In particular, formate ligands which are originate from partial pyrolysis of DMF participate in coordination bonds and provide electron pairs to Zn(II). The dinuclear repeating unit consists of two Zn(II), four bpe ligands and four adc ligands. Zn(II) is six-coordinated by two nitrogen atoms of bpeb ligands and four oxygen atoms of adc ligands. Especially, the double bonds of bpeb ligands in **2** are parallelly aligned to each other at a distance of 3.8 Å. According to Schmidt's Criteria,[2] the distance between olefins within the range of 3.6-4.1 Å is photoreactive. Hence, the C=C bonds of bpeb ligands in **2** undergo [2+2] cycloaddition reaction. When UV is irradiated to **2**, double bonds are converted into cyclobutane rings. Especially, bpeb ligands have two sites of double bond but only single dimerization is observed which is adjacent to Zn(II). The photo-dimerized MOF $[Zn_2(dimer)_2(adc)_3(fa)]$ (**3**, dimer = (*E*)-4,4'-((1*R*,2*S*,3*R*,4*S*)-3,4-diphenylcyclobutane-1,2-diyl)bis(cinnamylbenzene)) was confirmed by ^{1}H nuclear magnetic resonance and single crystal X-ray diffraction analyses.

References

[1] G. K. Kole, J. J. Vittal, Solid-state reactivity and structural transformations involving coordination polymers, *Chem. Soc. Rev.*, **2013**, *42*, 1755-1775.

[2] G. M. J. Schmidt, Photodimerization in the solid state, *Pure Appl. Chem.*, **1971**, *27*, 647-678.

Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Formation of Zn(II) Supramolecular Isomers and Their Photoreactivity

Jaewook An, Dong Hee Lee, In-Hyeok Park*

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Supramolecular isomers have a same chemical formula but more than one crystal structure in coordination polymers (CPs) and metal-organic frameworks (MOFs).[1] Here we report the significant correlation of solvents, coordination environments, and photoreactivity between two Zn(II) supramolecular isomers. A 1D zigzag CP, [Zn(bpe)(adc)$_2$] (**1**) is synthesized under solvothermal reaction of $Zn(NO_3)_2{\cdot}6H_2O$, 1,2-bis(4-pyridyl)ethylene (bpe), and 1-adamantanecarboxylic acid (Hadc) in a mixture of dimethylacetamide (DMA) and H_2O. The mononuclear repeating unit in **1** consists of one Zn(II) atom, two bpe ligands, and two adc ligands. Zn1 atom is pseudo-tetrahedrally coordinated by two nitrogen atoms of bpe ligands and four oxygen atoms of adc ligands. On the other hand, a 1D railroad CP, [Zn(bpe)(adc)$_2$] (**2**) is synthesized by same reaction condition except dimethylformamide (DMF) instead of DMA. The dinuclear repeating unit in **2** consists of two Zn(II) atoms, four bpe ligands, and four adc ligands. Zn1 is octahedrally coordinated by two nitrogen atoms of bpe ligands and four oxygen atoms of adc ligands. Especially, the double bonds of bpe ligands in **2** are parallelly aligned to each other at a distance of 3.6 Å. According to Schmidt's Criteria,[2] while the distance of olefins is within the range of 3.6-4.1 Å, olefins can be photo-dimerized by UV irradiation. ^{1}H nuclear magnetic resonance (NMR) spectrum of the crystals obtained after irradiation of **1** under UV for 48 h showed the formation of cyclobutane peaks at 5.3 ppm. For better understanding of the irradiated crystal structure, we attempted to receive suitable single crystals for single crystal X-ray diffraction analysis (SC-XRD). The X-ray crystal structure of the photodimerized CP [Zn(*rctt*-tpcb)(adc)$_2$] (**3**, *rctt* = *regio, cis, trans, trans*; tccb = 1,2,3,4-tetrakis(3'-carboxyphenyl)-cyclobutane) was finally confirmed by SC-XRD. To monitor the homogeneity of **1** and **2**, the powder X-ray diffraction (PXRD) patterns have also been investigated. The details will be presented at the poster section.

References

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[2] G. M. J. Schmidt, Photodimerization in the solid state, *Pure Appl. Chem.*, **1971**, *27*, 647-678.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-101**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Heteroatom-doped nanomaterials/core–shell nanostructure based electrocatalysts for the oxygen reduction reaction

NaHyun Park, Kang Hyun Park*

Department of Chemistry, Pusan National University, Korea

Recently, heteroatom doped core–shell nanostructures (HCSNs) have been widely used as superior electrocatalysts for the oxygen reduction reaction (ORR) owing to their enhanced ORR performance and stability under harsh environmental conditions. In this review, we provide the importance of HCSNs and explain how the ORR performance can be enhanced by various heteroatom dopants, such as nitrogen, sulfur, phosphorous, boron, and combinations of two or more heteroatoms. Various types of nitrogen doping were performed with different forms of nitrogen-containing organic compounds in CSNs, such as metal–organic frameworks, zeolitic imidazolate frameworks, and transition metals containing nitrogen sources, which have been used widely for the ORR because they form a high surface area, a facet surface structure, and reactive active sites in the presence of elements that are useful for the ORR catalytic activity. Furthermore, we briefly discuss the synthesis and fabrication of highly efficient ORR electrodes using a combination of di-, tri-, or multi-heteroatom-doped CSNs. Finally, we discuss the superior ORR activities of the HCSNs reported in recent literature and compare the activity with various reactive descriptors and the broad scope of these HCSNs for practical applications, along with their drawbacks and future demands.

Poster Presentation : **INOR.P-102**

Inorganic Chemistry

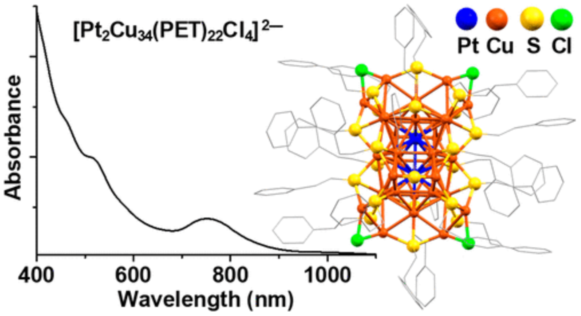
Event Hall FRI 11:00~13:00

[Pt2Cu34(PET)22Cl4]2–: An Atomically Precise, 10-Electron PtCu Bimetal Nanocluster with a Direct Pt–Pt Bond

Taeghwan Hyeon[*], **Guocheng Deng**

Division of Chemical & Biological Engineering, Seoul National University, Korea

Heteroatom-doped metal nanoclusters (NCs) are highly desirable to gain fundamental insights into the effect of doping on the electronic structure and catalytic properties. Unfortunately, their controlled synthesis is highly challenging when the metal atomic sizes are largely different (e.g., Cu and Pt). Here, we design a metal-exchange strategy that enables simultaneous doping and resizing of NCs. Specifically, [Pt2Cu34(PET)22Cl4]2– NC, the first example of a Pt-doped Cu NC, is synthesized by utilizing the unique reactivity of [Cu32(PET)24Cl2H8]2– NC with Pt4+ ions. The single-crystal X-ray structure reveals that two directly bonded Pt atoms occupy the two centers of an unusually interpenetrating, incomplete biicosahedron core (Pt2Cu18), which is stabilized by a Cu16(PET)22Cl4 shell. The molecular structure and composition of the NC are validated by combined experimental and theoretical results. Electronic structure calculations, using the density functional theory, show that the Pt2Cu34 NC is a 10-electron superatom. The computed absorption spectrum matches well with the measured data and allows for assignment of the absorption peaks. The calculations also rationalize energetics for ligand exchange observed in the mass spectrometry data. The synergistic effects induced by Pt doping are found to enhance the catalytic activity of Cu NCs by ~300-fold in silane to silanol conversion under mild conditions. Furthermore, our synthetic strategy has potential to produce Ni-, Pd-, and Au-doped Cu NCs, which will open new avenues to uncover their molecular structures and catalytic properties.


$[Pt_2Cu_{34}(PET)_{22}Cl_4]^{2-}$
Pt
Cu
S
Cl
Absorbance
400
600
800
1000
Wavelength (nm)

Poster Presentation : **INOR.P-103**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

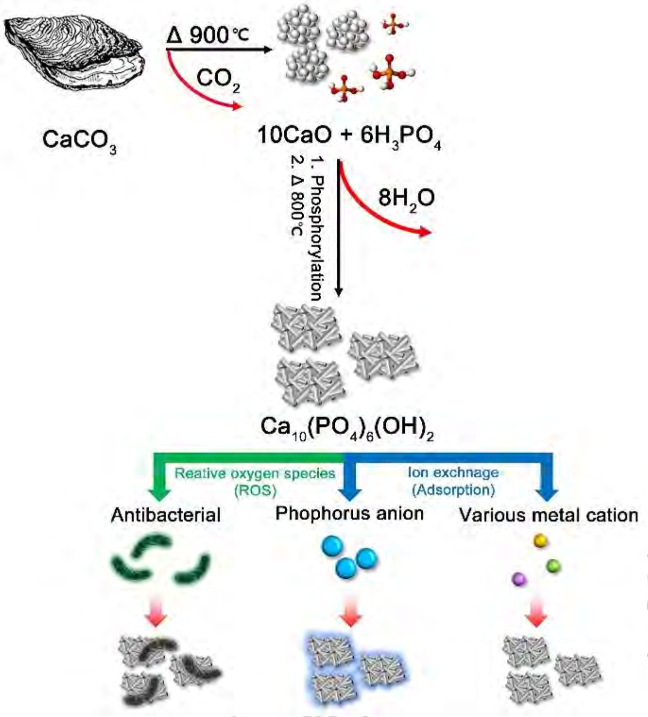
Removal of Various Hazardous Materials Using a Multifunctional Biomass-Derived Hydroxyapatite (HAP) Catalyst and Its Antibacterial Effects

Kyeongmun Park, **Kang Hyun Park**[1,*]

Department of Chemistry, Pusan National University, Korea

[1]*Department of Chemistry, Pusan National University, Korea*

In the present study, oyster shells, a cause of environmental pollution, were employed effectively to synthesize hydroxyapatite (HAP) by facile oxidation and phosphorylation. The ability of HAP to adsorb various metal cations and inhibit bacterial growth was validated. The biomass-derived HAP catalyst exhibited high metal cation adsorption in water at room temperature and under various acidic conditions (M = Cr, Mn, Ni, Cu, Cd, Ba, and Pb). HAP was demonstrated to have a maximum removal efficiency of 92.8% for the heavy metal Pb. Even under different pH conditions, HAP was demonstrated to be effective for the removal of three harmful heavy metals, Cr, Cd, and Pb, with a particularly high removal efficiency demonstrated for Pb under all conditions (average removal efficiency of Cr: 63.0%, Cd: 59.9%, and Pb: 91.6%). In addition, HAP had a significant influence on phosphate ion adsorption in aqueous solution, eliminating 98.1% after 3 min. Furthermore, biomass-derived HAP was demonstrated to have significant antibacterial activity against *E. coli* and *S. aureus* (5 mM: 74% and 78.1%, 10 mM: 89.6% and 96.0%, respectively).


CaCO3
Δ 900℃
CO2
10CaO + 6H3PO4
1. Phosphorylation
2. Δ 800℃
8H2O
Ca10(PO4)6(OH)2
Reative oxygen species
(ROS)
Ion exchnage
(Adsorption)
Antibacterial
Phophorus anion
Various metal cation

Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Vitamins Could Regulate Matrix Metalloproteinase-2 Activity

Eungchan Kim, Jae-Hyun Kim, Nak Han Jang, Hyunjung Kim, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) are known as many pathological indicators, including Alzheimer's disease (AD). Among them, high levels of MMP-2 has been observed in AD patients' brain. Moreover, MMP-2 could directly degrade amyloid precursor protein (APP) and amyloid-β (Aβ), which are considered as the main risk factors of AD. On this account, MMP-2 has been suggested to be related to the occurrence and progression of AD. In this study, we investigated the effect of both fat and water soluble vitamins [i.e., retinol (vitamin A), pyridoxamine (vitamin B6), ascorbic acid (vitamin C), and cholecalciferol (vitamin D3)] on the activity of MMP-2. The interactions between vitamins and MMP-2 were identified through docking simulations and the enzymatic activity of MMP-2 in the presence of vitamins was determined through zymography. As a result, vitamins could inhibit the activity of MMP-2 by interacting with the enzyme near the active site. Investigating the relationships between biomolecules, such as vitamins, and MMP-2 can help understanding the influence of MMP-2 on the etiology of AD.

Poster Presentation : **INOR.P-105**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Regulation of Matrix Metalloproteinase-9 Activity by Vitamins

Eungchan Kim, Jae-Hyun Kim, Nak Han Jang, Hyunjung Kim, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) have been proposed as pathological indicators for various diseases including Alzheimer’s disease (AD), intervertebral disc degeneration, and restenosis. Among MMP family, MMP-9 has been revealed to be associated with AD because its increased level was observed in the brain tissue of AD patients. In addition, MMP-9 degrades both amyloid precursor protein (APP) and amyloid-β (Aβ) which could form toxic aggregates causing AD. In this study, we will examine the influence of multiple natural products (e.g., vitamins) on MMPs’ peptide degrading ability as well as propose the mechanisms how those biomolecules affect the activity of MMPs under various conditions (e.g., stoichiometry) using biochemical and biophysical methods (i.e., zymography, colorimetric assay, docking simulations). Our overall investigation from multiple experiments could provide better insight into the study of the MMP-9 which could cleave Aβ, related to AD pathology.

Poster Presentation : **INOR.P-106**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Coordination of concanavalin A to xenobiotic metal ions

Chae Min Lee, Seung Jae Lee[1,*]

Department of Chemistry, Jeonbuk National University, Korea
[1]*Department of Chemistry and Institute of Molecular Biology and Genetics, Jeonbuk National University, Korea*

A practical method for detecting and concentrating viruses is essential for controlling disease outbreaks. Highly sensitive and reliable techniques that can monitor small amounts of viral copies are not applicable to date. The properties of lectins allow them to bind to carbohydrates which is crucial in detecting receptor glycoprotein interactions. The structural and functional studies of concanavalin A (ConA), an intensively investigated lectin, proved that it interacts with glucose and mannose. X-ray crystallography confirmed that ConA consists of two b-sheets and a short a-helix as a form of metalloprotein that is housed with Mn^{2+} and Ca^{2+} in the loop region. We have discovered the details of the interactions between ConA and human norovirus (HuNoV), that can facilitate the development of a sensitive detection method. Biophysical studies including hydrogen/deuterium exchange mass spectrometry (HDX-MS) and surface plasmon resonance (SPR) demonstrated that the metal coordination domain (MCD) is crucial for forming hydrogen bonds with carbohydrates. The specific hydrogen bonds were generated through carbohydrate binding domain (CBD) including Tyr, Asp, and Arg residues. Previous biophysical studies have proposed that diverse environments with identical compositions of ConA and carbohydrates may still have different dissociation constants (K_ds) due to its complexation. The majority of interactions for the dimer are hydrogen bonds between two b-strands but the trimeric complex is regulated by the coordination with Cd^{2+}. This study shows that ConA can generate diverse complexes including monomers, dimers, trimers, and tetramers based on the acidity, buffer conditions, and xenobiotic metal ions.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Electron transfer mechanisms of MMOR, a reductase of soluble methane monooxygenase

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[1]*Department of Chemistry and Institute of Molecular Biology and Genetics, Jeonbuk National University, Korea*

Methane (CH_4) has a higher heat capacity than carbon dioxide (CO_2), and its impact is more critical to global warming. Its C-H activation energy (104.0 kcal/mol) is high and the hydroxylation from methane to methanol can provide valuable information for the conservation of nature. Soluble methane monooxygenase (sMMO) converts methane to methanol under ambient conditions. Therefore, the elucidation of its catalytic cycle is a key issue for scientists. Our research team has studied these enzymatic mechanisms and reports two complex protein structures and an electronic environment. sMMO oxidizes methane to methanol using at least three proteins, including the regulatory protein (MMOB) and reductase (MMOR). The MMOH-MMOB complex (*Nature* 2013) provides details about the hydroxylation reactions that occur inside MMOH by MMOB's allosteric effects. Unfortunately, the MMOH-MMOR complex and the entire sequence of MMOR structures has not been reported to date. In this presentation, we investigated the structure of MMOR and analyzed the first X-ray structure of MMOR FAD-binding domain (MMOR-FAD) to understand the electron transfer routes. The six β-strands with two α-helices generated a β-barrel. The sidechains of hydrophobic amino acids are oriented toward the inner space, and the sidechains of hydrophilic amino acids are oriented toward the solvent-accessible area. We realized that four hydrogen bonds to the FAD cofactor could be the electron transfer pathways, and mutational studies identified that Tyr160 is a key residue for its catalytic cycle in sMMO.

Poster Presentation : **INOR.P-108**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Coordination selectivity of cobalt ion to the classical zinc finger, PARIS

Yunha Hwang, Seung Jae Lee[1,*]

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The major transcriptional and translational regulators in eukaryotes and prokaryotes are zinc finger (ZF) proteins. The structural and functional aspects of these proteins have been intensively investigated, owing to their crucial importance in the Central Dogma. ZF proteins have a distinct feature as metalloproteins, because the specific secondary folding in local ZF domains is generated in the presence of zinc ions. ZF domains consisting of Cys and His residues can function independently in many cases, and the biochemical aspects of these ZF domains are widely studied, to understand their specific roles. This presentation demonstrates the possible application of zinc fingers for recycling of metal ions, to obtain selective cobalt ions using induced E. coli systems. There have been precedent approaches that have attempted to understand the coordination of heterometal ions such as ferrous, ferric, cobalt, copper, and others through purified zinc finger domains, but this study provides possible applications of zinc fingers in biological systems. A classical three-zinc finger domain (PARIS_ZF2-4) from the protein expressed in the brain, PARIS, was investigated to understand metal coordination. The results provided the valuable information that PARIS_ZF2-4 selectively coordinates to cobalt in the E. coli system. Iron and copper cannot replace metal ions in PARIS, although iron improves the expression level of zinc-bound PARIS_ZF2-4. In addition, PARIS_ZF2-4 was expressed and purified for basic characterization and showed cobalt-binding abilities.

Poster Presentation : **INOR.P-109**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Back charge transfer from MCl_6 anions to tetrathiafulvalene in tetrathiafulvalene radical salt and its effect on electrical conductivity

Yoolim Ahn, Hee Cheul Choi*

Department of Chemistry, Pohang University of Science and Technology, Korea

TTF_3MCl_6 (M=In, Sb) series were developed for an ideal platform to investigate on the effect of metal of MCl_6^{3-} on the electrical conductivity of TTF_3MCl_6 complexes. It is only recent that the electrical conductivity of the TTF radical salt is contributed not only by the TTF radicals but also by the back charge transfer from the counter ion. However, this effect is rarely investigated since the crystal structure of the complex is also changed when the counter ion changed, making it difficult to clearly see the effect of back charge transfer from different anions. Thus, it is important to develop a platform system that allows systematic studies on the conductivity changes according to the change of back charge transfer power of the anions without significant structural difference. As such system, TTF_3MCl_6 (M=In, Sb) series were successfully synthesized by a UV light-induced one-pot reaction where TTF oxidation and formation of MCl_6^{3-} occurred sequentially. The type of center metal can be easily controlled by changing the metal chloride source. In isostructural TTF_3InCl_6 and TTF_3SbCl_6, the intermolecular interaction between MCl_6^{3-} and TTF induces back charge transfer, which were confirmed by the crystal structure and spectroscopic analyses. Despite the similar crystal structure, TTF_3InCl_6 shows 3-orders of magnitude higher electrical conductivity compared to TTF_3SbCl_6. According to the cyclic voltammograms (CV) and electron spin resonance (ESR) spectra, the increased conductivity turned out to owe to the higher degree of back charge transfer from MCl_6^{3-} in TTF_3InCl_6 compared to TTF_3SbCl_6, which is due to the lower electronegativity of In than Sb. Our results suggest that anions have an immense effect on the conductivity of the complex through back charge transfer.

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Crystalline imine-based polymer thin film growth by chemical vapor deposition

<u>YeLim Son</u>, Hee Cheul Choi[1,*], Myeonggeun Choe[2]

Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*
[2]*Chemistry, Pohang University of Science and Technology, Korea*

Covalently linked polymers in a large-area and highly-uniform thin film are promising materials for electronic devices with thermal stability, flexibility, and solution processability. There have been attempts to synthesize the polymer thin film by chemical vapor deposition (CVD) which is an important tool for high-quality thin film growth. However, most attempts were limited to radical reactions, requiring complex systems using oxidants or initiators. Herein, we present our recent achievements of crystalline imine-based polymer thin film by CVD without any oxidants or initiators. We demonstrate a CVD method for inducing vapor-phase imine-condensation reaction for producing imine-based polymer, a prototypical polymer. We offer the growth model of large-area imine-based polymer thin films from vapor-phase reaction between triformylbenzene (TFB) and phenylenediamine (PDA) molecules. Further, we verify the effect of reaction temperature and water vapor on crystallinity of polymer thin films. We believe that our study would contribute to the development of a novel method and understanding of growth mechanism for crystalline polymer thin films.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Chemical vapor deposition of edge-on oriented 2D conductive metal-organic framework thin films

Myeonggeun Choe, Hee Cheul Choi[1,*], Sarah Sunah Park[1,*]

Chemistry, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Chemical vapor deposition (CVD) method opens up new opportunities for incorporating metal-organic frameworks (MOFs) into actual devices. While there are some MOFs synthesized by CVD, they are still limited to insulating MOFs. Therefore, a novel approach is demanded for a conductive two-dimensional metal-organic framework (2D MOF). In this presentation, we present a one-step all-vapor-phase CVD method for Cu3(HHB)2 (Cu3(C6O6)2, HHB=hexahydroxybenzene) thin-film synthesis, one of the conductive 2D MOFs. We will specially discuss the formation of large-area and highly-oriented Cu3(HHB)2 thin films with very good crystallinity and unique edge-on orientation. Further, we also discuss a stepwise growth mechanism and intermediate species of the vapor-phase reaction. Cu3(HHB)2 thin film-based microdevices were fabricated by an e-beam lithography (EBL) and show electrical conductivity, σ = 1.76 S/cm. Our study will not only propose a novel method for 2D c-MOF thin film synthesis but also contribute to the fundamental mechanism study of a vapor phase reaction that has hardly been studied.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

THF-solvated electrons via potassium dissolution

Changmin Choi, Hee Cheul Choi[1,*]

Department of chemistry, Pohang University of Science and Technology, Korea

[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Free electrons are responsible for many essential properties including electricity of metals and various chemical reactions including electrochemical redox reactions. Out of metals, free electrons are quite rare to exist. Solvated electrons, one potential form of free electrons, have been known as a key system for elucidating the mechanism of redox reactions in solution such as hydrogen evolution reaction and birch reduction. Recently, it has been reported that the solvated electrons are formed when potassium dissolves in liquid ammonia at low temperature. However, considering the harsh condition required for liquid ammonia, it is highly demanded to find milder environments allowing the formation of solvated electrons for its practical use. In this presentation, we discuss our recent achievements of the formation of solvated electrons by dissolving potassium metal in a tetrahydrofuran (THF) solution. We will discuss in detail about the identity of the solvated electrons studied by mass spectroscopy as well as its doping applications for the formation of fullerene superconductor and semiconductor doping.

Poster Presentation : **INOR.P-113**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Highly Efficient Platinum(II) Complexes for Application to White Organic Light-Emitting Diodes(WOLEDs)

Youngjin Kang*, Dain Cho, Hyeon Ji Kim, Sujin Lee, Sang Geun Jeon

Division of Science Education, Kangwon National University, Korea

Three cyclometalated Pt(II) β-diketonate compounds with sky-blue to green phosphorescence are prepared by modifying the substituents of the 2′,6′-dimethoxy-2,3′-bipyridine (OMe_2pypy, C^N) chelate ligand. These molecules have the general formula Pt(C^N)(O^O), where O^O = acetylacetonate; one is unsubstituted (1), one possesses a trimethylsilyl (TMS) substituent (2), and the other is substituted with dimesitylboron ($BMes_2$) (3). The intermolecular interactions of 2 are greater than those of 1 and 3, based on color mapping and surface area results from Hirshfeld analyses. Time dependent density functional theory calculations reveal that the electronic transitions of monomeric 1 and 3 are predominantly intra-ligand or ligand-toligand charge transfer mixed with metal-to-ligand charge transfer transitions, while for the dimeric forms, dimeric 2, an additional strong metal–metal-to ligand charge transfer transition is observed. White organic light-emitting diode (WOLED) devices using an 1,3-bis(N-carbazolyl)benzene (mCP) or mCP:TSPO1(diphenyl[4-(triphenylsilyl)phenyl]phosphine oxide) mixed host and 1–3 as dopants are fabricated. With a dopant concentration of 20 wt% in the emissive layer, compound 2 exhibited bright yellow–green emission with a maximum external quantum efficiency (EQE) of 24.9%. This result corresponds to one of the highest EQEs among the reported C^N chelated Pt(II) β-diketonate-based WOLEDs.

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

New homochiral coordination polymers constructed from Alanine derivatives

Jihyun Lee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Synthesis of crystalline materials with noncentrosymmetric (NCS) structures is not easy because the natural system prefers to crystallize in highly symmetric space groups. However, the demand for compounds with NCS structures has been increasing continuously owing to the materials' industrially useful properties such as ferroelectricity, piezoelectricity, pyroelectricity, and second harmonic generation (SHG) properties. Recently, we have found that introducing chiral structure-directing agents is a very good strategy to systematically synthesize crystalline materials with NCS structures. In this work, two homochiral metal-organic coordination polymers (CPs) have been hydrothermally synthesized by using alanine derivative chiral ligands. The title compounds, **Cd(*S*)** and **Zn(*S*)**, have two chiral ligands and two achiral pillar ligands centered on the 5-and 6-coordinate metal polyhedral dimers. Single crystal X-ray diffraction suggests that the structures of the title CPs crystallize in the triclinic NCS space group, *P*1. The unique three-dimensional structures were formed via intermolecular hydrogen bonding and intramolecular π-π stacking interactions. Powder SHG measurements using 1064 nm laser reveals that the title compounds have SHG efficiency of ca. 2 times that of KH_2PO_4.

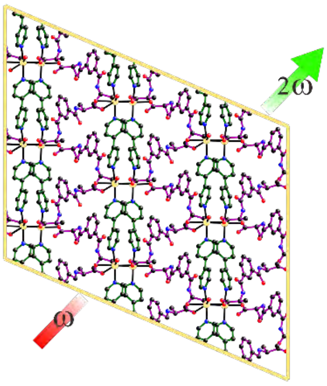


Fig. 1 Ball-and-stick model and SHG active representation of **Cd(*S*)** in the *bc*-plane. (yellow, Cd; black, C; blue, N; red,O and H atoms were omitted for clarity.)

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Characterization of a Series of Alkali Metal Gallium Iodate Fluorides

Myung-Ho Choi, Kang Min Ok[1,*]

Division of Chemistry, Sogang University, Korea

[1]*Department of Chemistry, Sogang University, Korea*

Three gallium iodate fluoride multi-anion complexes have been prepared through hydrothermal reactions. Ga^{3+} cation often reveals an octahedral coordination environment with oxide ligands. And the fluoride source not only has an excellent ability to dissolve substances that are poorly soluble in water but also could be applied to extend band gaps in solid-state materials. In addition, iodates have received much attention due to the optical utilization of lone pair electrons. Single crystal X-ray diffraction analysis suggests gallium fluoride octahedra are connected by adjacent gallium fluoride units and other anions. Depending on the size of alkali metal cations, the composition of the obtained complexes varies. Li-complex crystallizing in the monoclinic space group, $P2_1/n$, exhibits a two-dimensional layered structure with infinitely extended $[Ga_2F_4(IO_3)_6]$ units bridged by (IO_3) groups. The structures of isostructural Rb and Cs-complexes crystallizing in the orthorhombic space group, *Pnma*, reveal infinite 1D chains that are alternately bridged by iodates. The multi-anion complexes have been fully characterized by various spectroscopic and thermogravimetric analyses along with the density functional theory calculations.

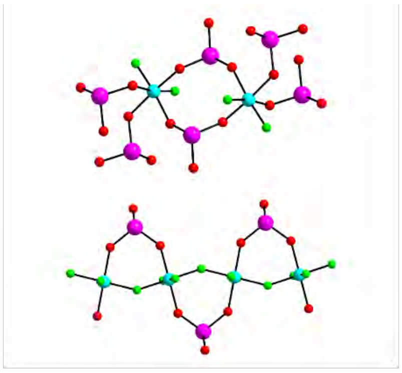


Figure. Ball-and-stick representation of gallium fluoride iodate unit of Li-complex (top) and Rb, Cs-complexes (bottom) (cyan, Ga; pink, I; green, F; and red, O).

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

New noncentrosymmetric hybrid niobium oxyfluorides templated by chiral amino acids

Jihyeon Moon, Kang Min Ok[1,*]

Chemistry, Sogang University, Korea

[1]*Department of Chemistry, Sogang University, Korea*

Large-sized colorless crystals of niobium oxyfluorides with noncentrosymmetric (NCS) structures have been synthesized by a slow evaporation method using chiral amino acid templates. Single crystal X-ray diffraction suggests that the title compounds crystallize in the NCS nonpolar space group, $P2_12_12$. The inter- and intra- hydrogen bonding interactions between protonated chiral amino acid cations and distorted niobium oxyfluoride octahedra result in pseudo three-dimensional structures. The title compounds exhibit very large birefringence (Δn_{obv} = 0.19–0.199 @589.3 nm) due to the stacking of benzene rings in chiral amino acids aligned along the b-axis. Further characterizations such as thermal properties, various spectroscopic analyses, stability in diverse solvents, powder second-harmonic generation properties, and electronic structure calculations are also presented.

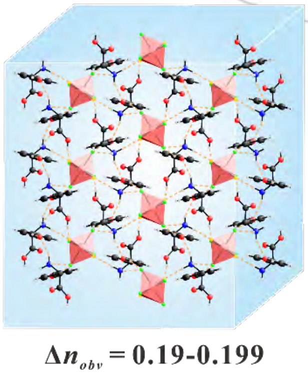


Fig. 1 Stacking of benzene rings in chiral templates leads to large birefringence of the title compounds.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

The Catalytic Property of Zinc(II) Complexes Supported by *N,N'*-Aminomethylpyridine and *N,N'*-Aminomethylquinoline Derived Ligands

Jaegyeong Lee, Hyosun Lee[*]

Department of Chemistry, Kyungpook National University, Korea

Zinc(II) complexes, namely **[L_nZnCl_2]** (L_n = L_A–L_D) supported with *N*-substituted *N*,*N'*-aminomethylpyridine and *N*,*N'*-aminomethylquinoline derived ligands, such as 2-(piperidin-1-ylmethyl)pyridine (L_A), 4-(pyridin-2-ylmethyl)morpholine (L_B), 2-(piperidin-1-ylmethyl)quinoline (L_C) and 4-(quinolin-2-ylmethyl)morpholine (L_D), were synthesized and characterized. All complexes were characterized by ^{1}H-NMR, ^{13}C-NMR, IR, elemental analyzer, and single crystal X-ray diffraction. The catalytic properties of these complexes toward the polymerization of *rac*-lactide (LA) in the presence of initiator LiO^{i}Pr, LiMe, and LiCl were investigated at two different temperatures of 0 ^{o}C and 25 ^{o}C.

Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Zn(II) complexes bearing thiophenyl and furyl derived C_2-symmetric ligands: Synthesis, characterization, urease inhibitory activities and molecular docking

Saira Nayab, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

A series of Zn(II) complexes supported with C_2-symmetric propylene-based *N*,*N*-diamines ligands, $L^1 - L^4$, where $\mathbf{L^1}$ is 2,2-dimethyl-N^1,N^3-bis(thiophen-2-ylmethyl)propane-1,3-diamine, $\mathbf{L^2}$ is N^1,N^3-bis(thiophen-2-ylmethyl)propane-1,3-diamine, $\mathbf{L^3}$ is N^1,N^3-bis(furan-2-ylmethyl)-2,2-dimethylpropane-1,3-diamine, and $\mathbf{L^4}$ is N^1,N^3-bis(furan-2-ylmethyl)propane-1,3-diamine, have been synthesized and characterized. Structural studies revealed that $\mathbf{[L^nZnCl_2]}$ ($L^n = L^2$ and L^4) adopted distorted tetrahedral geometries around the metal center. The synthesized Zn(II) complexes were tested *in vitro* for their urease inhibitory potential against *Jack bean urease* (JB urease) and *Bacillus pasteurii urease* (BP urease). Zn(II) complexes bearing thiophenyl pendant moieties, $\mathbf{[L^1ZnCl_2]}$ and $\mathbf{[L^2ZnCl_2]}$, exhibited prominent inhibitory potential against JB urease (IC_{50} = 25.15±1.99 and 12.5±0.15 μM), and BP urease (IC_{50} = 18.05±1.01 and 9.10±0.12 μM) compared to the standard thiourea (IC_{50} =10±0.52 and 8.20±0.90 μM). Additionally, molecular docking confirms the probable binding modes of the active complexes into the crystal structure of JB urease.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Cadmium(II) Complexes Containing *N,N'*-Bidentate Aminomethylquinoline and Aminomethylpyridine Derived Ligands: Synthesis, Structure and Polymerization of *rac*-Lactide

Yerim Cho, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized a new series of Cd(II) complexes, namely **[L_nCdBr_2]** by the reaction of **[$CdBr_2·4H_2O$]** with ligands **L_n** (L_n = L_A – L_D) in which L_n is 2-(piperidin-1-ylmethyl)pyridine, 4-(pyridin-2-ylmethyl)morpholine, 2-(piperidin-1-ylmethyl)quinoline and 4-(quinolin-2-ylmethyl)morpholine, respectively. All synthesized complexes were analyzed by various spectroscopic methods such as ^{1}H-NMR, ^{13}C-NMR, IR, elemental analyzer and single crystal X-ray diffraction. The catalytic activities of Cd(II) complexes toward the polymerization of *rac*-Lactide (LA) in the presence of LiO^iPr were investigated at 0 °C and 25 °C.

Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Spin crossover behavior in Fe(III) complexes with halogen-substituted Schiff-base ligand: structure and magnetic property

Ahrim Jeong, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

The development of spin crossover (SCO) materials continues to generate a great deal of interest from both fundamental and applied perspectives because of their potential and/or practical applications for data storage devices, molecular switches, displays and sensors. Recently, novel iron(III) complex, [(3,5-Cl-qsal)$_2$Fe](SO$_4$H)•2CH$_3$OH (**1•2MeOH**) has been prepared by using iron(III) species with 3,5-dichloro-*N*-(8-quinolyl)salicylamine (3,5-Cl-Hqsal) in an aerobic condition. The crystal structures of iron(III) complexes were determined by single crystal X-ray diffraction at 100 K and 298 K, respectively. For **1•2MeOH**, the average F–N/O distances are 1.9223(15) Å at 100 K and 1.9153(16) Å at 298 K and related to low spin state. On the other hand, the average F–N/O distances of desolvated complex **1** are 1.9291(8) and 2.0180(12) Å at 100 and 298 K, and related to low spin and high spin state, respectively. **1** shows spin crossover behavior about 200 K and that is responsive to CO$_2$ adsorption. In this poster, we will present the detailed preparation, crystal structure, magnetic properties.

Poster Presentation : **INOR.P-121**

Inorganic Chemistry

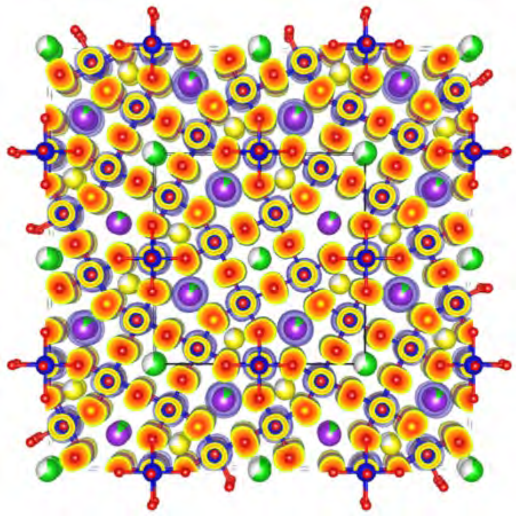
Event Hall FRI 11:00~13:00

Second Harmonic Generation Properties of a Niobium Oxide-based Tetragonal Tungsten Bronze

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Discovering solid-state materials with extended structures has drawn numerous academic attentions owing to their many intriguing structure-related physical, chemical, and optical properties. Among many characteristics, materials with high-performance second-harmonic generation (SHG) can effectively produce a new coherent frequency doubled-light from the input light. Here, we present synthesis, structure determination, and characterization of a nonstoichiometric tetragonal tungsten bronze. The title compound has been successfully synthesized by a conventional solid-state reaction. The structure of the reported tungsten bronze features a three-dimensional framework consisting of corner-sharing NbO_6 polyhedra. Remarkably, the title compound reveals extremely large SHG efficiencies of about 71.5 times that of KH_2PO_4 and the type-I phase-matching behavior. To the best of our knowledge, the title compound exhibits the strongest SHG efficiencies among the reported tungsten bronze structures owing to the presence of extremely large structural distortion in polyhedra.



129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

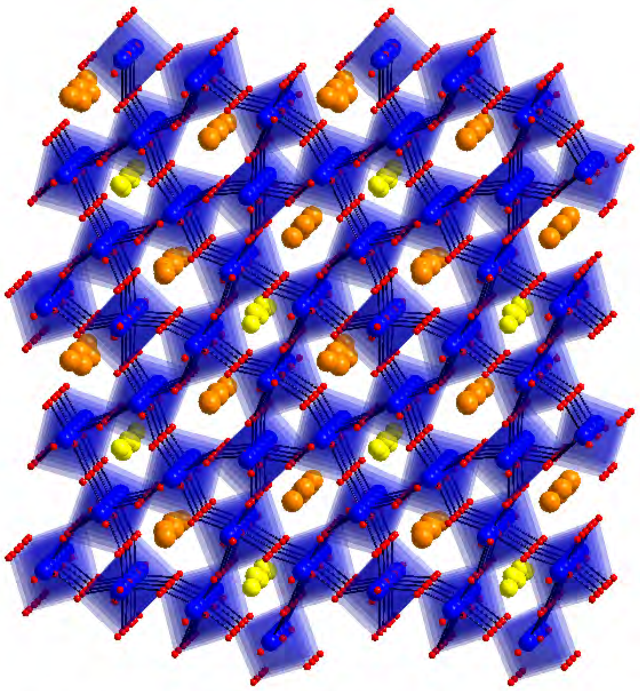
Event Hall FRI 11:00~13:00

Structural distortions and Second-Harmonic Generation Properties of Tungsten Bronze Oxides

Yejin Pi, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Discovering the nonlinear optical (NLO) materials with strong second harmonic generation (SHG) is still an on-going challenge. Generating a large polarization is considered as a good strategy to obtain high performance NLO materials. Tungsten bronze (TB) oxides are a good candidate for NLO applications because of their unique structural characteristics such as distorted octahedra aligned along a specific axis. Herein, we present synthesis, structure, and characterization of new TB oxides materials. In particular, we have observed a significant structural difference between the transition metal doped-TB and undoped-TB oxides. The doped-TB shows also an enhancement of the SHG response compared to that of the undoped-TB. The observed SHG for the reported materials are explained by the dipole moment calculations.



Poster Presentation : **INOR.P-123**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

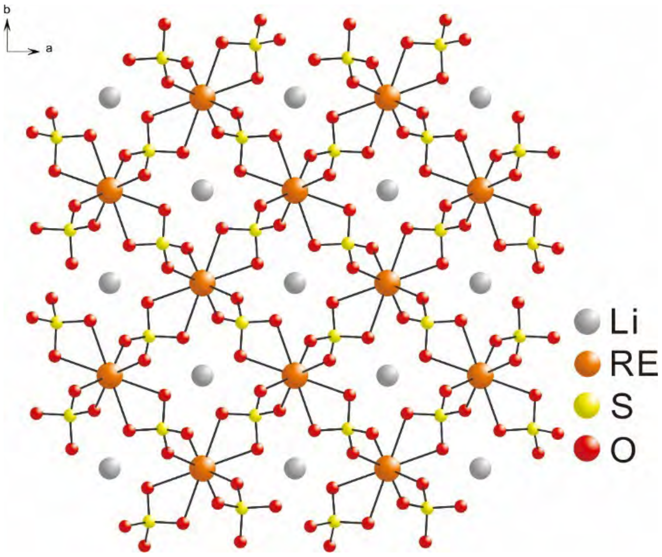
Solid-state synthesis, structure determination, and characterization of a series of lithium rare-earth metal sulfates

Sunghwan Cho, Kang Min Ok[1,*]

Department of chemistry, Sogang University, Korea

[1]*Department of Chemistry, Sogang University, Korea*

Three new ternary lithium rare earth metal sulfates have been synthesized by high temperature solid state reactions and solvothermal reactions. The reported materials crystalizing in the noncentrosymmetric (NCS) nonpolar tetragonal space group, P-4n2 (no. 118) exhibit three-dimensional structures consisting of REO_8, LiO_4, and SO_4 groups. Ultraviolet-visible diffuse reflectance spectra and density functional theory calculations indicate that the reported materials exhibit very large band gaps of ca. 6.7 eV, which are wide enough to be transparent to light under 185 nm. The frameworks of the sulfates reveal high thermal stabilities of up to 873~1073 K depending on the constituting rare earth cations. IR spectra show absorption bands originating from SO_4, REO_8, and LiO_4 groups. Powder second-harmonic generation (SHG) measurements reveal that the sulfates with NCS structures have rather mild SHG responses of similar to that of KH_2PO_4 and are non-phase matchable. Detailed synthetic procedures, crystal structures, and full characterizations of the new sulfates are presented.


b
a
Li
RE
S
O

Poster Presentation : **INOR.P-124**

Inorganic Chemistry

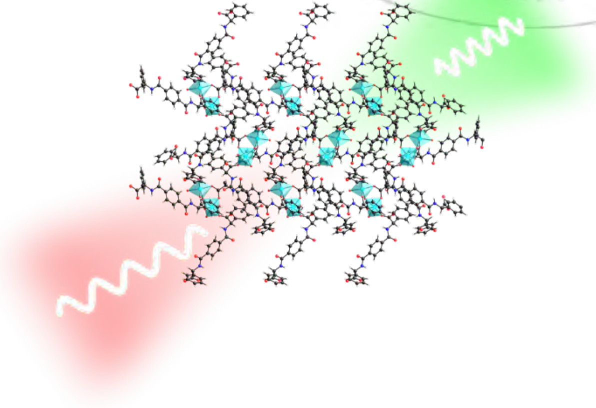
Event Hall FRI 11:00~13:00

Hydrothermal Synthesis, Crystal Structure Determination, and Characterizations of Noncentrosymmetric Chiral Zn-Coordination Polymers

Minju Lee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

In this research, we have successfully synthesized two Zn-based noncentrosymmetric (NCS) chiral coordination polymers through mild hydrothermal reactions by introducing chiral organic ligands. Compounds RZn and SZn crystallized in the monoclinic polar space group, $P2_1$. Interestingly, because of the π-π and hydrogen bonding interactions between the two types of layers, RZn and SZn show rare two-dimensional bilayer structures that are extending along the *bc* plane. The induced chirality of RZn and SZn is clearly confirmed by the inverted signals observed in the solid-state circular dichroism spectra. Compounds RZn and SZn with NCS structures reveal SHG efficiencies of about 1.5 times that of KH_2PO_4. Other characterizations such as spectroscopic and thermal analyses will be also discussed.



Poster Presentation : **INOR.P-125**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

A Nonheme Iron(III)-Peroxo Intermediate: an Unprecedented Electrophilic Reactivity

Wenjuan Zhu, Yong-Min Lee[1], Mi Sook Seo[2], Wonwoo Nam[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Institute of Nano & BioTechnology, Ewha Womans University, Korea*

A mononuclear nonheme iron(III)-peroxo intermediate, $[Fe(III)(O_2)(13\text{-}TMC)]^+$ (**1**), was synthesized and characterized by various spectroscopic techniques, such as CSI-MS, EPR, Mössbauer, XAS, and resonance Raman (rRaman) spectroscopies. The spectroscopic results of **1** supported a high-spin $S = 5/2$ Fe(III) species binding an O_2-unit. Surprisingly, **1** showed an electrophilic reactivity in hydrogen atom (H-atom) abstraction and oxygen atom transfer (OAT) reactions. In the H-atom reaction, a kinetic isotope effect (KIE) value of 5.8 was obtained in the oxidation of 9,10-dihydroanthracene. In the OAT reaction, a negative ρ value of –0.61 in Hammett plot was determined in the oxidation of *para*-X-substituted thioanisoles. Remarkably, the electrophilic reactivity of **1** was observed in the oxidation of benzaldehyde derivatives, which was supported by a negative ρ value of –0.77 in Hammett plot and a KIE value of 2.2. To the best of our knowledge, the current study has provided the first example of a mononuclear nonheme iron(III)-peroxo complex with an unprecedented electrophilic reactivity in oxidation reactions.

Poster Presentation : **INOR.P-126**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Manganese(III)-Iodosylarene Porphyrin Adducts: Unprecedented High Reactivity in Oxidation Reactions

Lina Zhang, Yong-Min Lee[1], Mi Sook Seo[2], Wonwoo Nam[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Institute of Nano & BioTechnology, Ewha Womans University, Korea*

The reactivity of Mn(III)-iodosylarene porphyrin adducts, $[\mathrm{Mn^{III}(Porp)(ArIO)}]^+$, has been investigated in the C-H bond activation (hydrogen atom transfer; HAT) and oxygen atom transfer (OAT) reactions and compared with those of the corresponding $\mathrm{Mn^{IV}(Porp)(O)}$ complex. In HAT reactions, $[\mathrm{Mn^{III}(Porp)(ArIO)}]^+$ are capable of activating unactivated alkanes such as cyclohexane, and shows unique reactivities, such as a saturation behavier of reaction rates, a low kinetic isotope effect of ~1.5, and no porphyrin ligand effect on the reactivity. In OAT reactions, the sulfoxidation of *para*-X-substituted thioanisoles by $[\mathrm{Mn^{III}(Porp)(ArIO)}]^+$ affords a very unusual behavior in the Hammett plot. The mechanisms of the C-H bond activation and OAT reactions by $[\mathrm{Mn^{III}(Porp)(ArIO)}]^+$ are discussed as well. To the best of our knowledge, the present study reports the first example of highly reactive Mn(III)-iodosylarene porphyrin adducts with unprecedented reactivities in HAT and OAT reactions.

Poster Presentation : **INOR.P-127**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Acid-Promoted Oxidation of Substrates by Mononuclear Nonheme Iron(III)-Aqua Complexes

Madhuri Nilajakar, Yong-Min Lee[1], Shunichi Fukuzumi[2,*], Wonwoo Nam[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*

[2]*Department of Material and Life Science, Osaka University, Japan*

Acids are known to promote oxidation of substrates by metal-oxygen intermediates, such as metal-oxo, -hydroxo, -peroxo, -hydroperoxo, -superoxo and -aqua complexes. Binding of more than one acid molecule to metal-oxygen intermediates is expected to enhance the oxidation reactivity with the higher order dependence of the rate constant on the acid concentration than the first-order. Such non-linear acid promotion has so far been reported only for the acid-promoted oxidation of substrates by metal-oxo complexes. Herein we report that binding of not only one but also two triflic acid (HOTf) molecules to mononuclear nonheme iron(III)-aqua complexes, $[(\mathrm{dpaq})\mathrm{Fe}^{\mathrm{III}}(\mathrm{OH_2})]^{2+}$ (**1**: dpaq = 2-[bis(pyridin-2-ylmethyl)]amino-N-quinolin-8-yl-acetamidate) and $[(\mathrm{tdpaq})\mathrm{Fe}^{\mathrm{III}}(\mathrm{OH_2})]^{2+}$ (**2**: tdpaq = 2-(benzyl(pyridin-2-ylmethyl)amino)-N-(quinolin-8-yl)acetamide), results in enhancement of the oxidation reactivity of the iron(III)-aqua complexes to exhibit the first-order and second-order dependence of the rate constant on the HOTf concentration ([HOTf]). The rate constants of electron transfer by **1** and **2** exhibit the second-order dependence on [HOTF], whereas the rate constants of hydrogen atom transfer and oxygen atom transfer by **1** and **2** exhibit both the first-order and second-order dependence on [HOTf]. The dependence of the logarithm of the rate constants of acid-promoted oxidation reactions by **1** and **2** on the driving force of electron transfer was evaluated in light of the Marcus theory of outer-sphere electron transfer.

Poster Presentation : **INOR.P-128**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

N-Heterocyclic Carbene (NHC) Enhances Thermal Stability of Molecular-scale Thermoelectric Devices and Enables Consistent Seebeck Effect

Sohyun Park, Jeong Woo Jo, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

The Seebeck effect is an important physical phenomenon that enables the conversion of waste heat into electricity. According to a report from the European Union (EU), ~90 % of waste heat discharged from industrial processes falls into the temperature range up to ~573 K. The Seebeck effect can be realized with individual molecules or monolayers, but molecular thermoelectric devices usually cannot withstand such high temperature ranges. This is mainly due to the delicate feature of organic-electrode contact. Indeed, in the study of molecular thermoelectrics, the delicate feature of the sulfur atom in thiol—the most widely used anchor in introducing molecules onto the surface of electrode—has limited the applicable temperature range only up to 333 K. In this presentation, we show N-heterocyclic carbene (NHC) can be a robust anchor and leads to molecular junctions with consistent Seebeck coefficient under harsh thermal environments (heating temperatures up to 573 K), generating thermovoltage up to ca. |1900 microV|. Structural analysis indicates that the NHC anchor maintains without appreciable structural change under the thermal environments, whereas thiol degrades into unbound species and leads to deteriorated thermoelectric performance. Our work demonstrates NHC-based anchor chemistry can contribute to resolving the stability problem in energy conversion devices.

Poster Presentation : **INOR.P-129**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Dinuclear gold(I) complexes supported by a chelated phosphine

Yong-Joo Kim

Department of Chemistry, Gangneung-Wonju National University, Korea

God(I) complexes with a chelated phosphine ligand show interesting coordination behaviors such as Au-P linked monomeric, dimeric, and polymeric formation of gold(I) complexes and also exhibit inter or intramolecular Au - Au aurophilic interactions depending on the phosphinyl substituents. In this context, we have interested in gold(I) complexes supproted by a chelated ligand with functional substituents which can reveal potential Au-Au interactions and be applied to the heterocycle formation. In this work, we have examined synthesis and structural analysis of new monomeric or polymeric gold(I) complexes supported by a ferrocenyl diphophine ligand. Detail explanation will be discussed.

Poster Presentation : **INOR.P-130**

Inorganic Chemistry

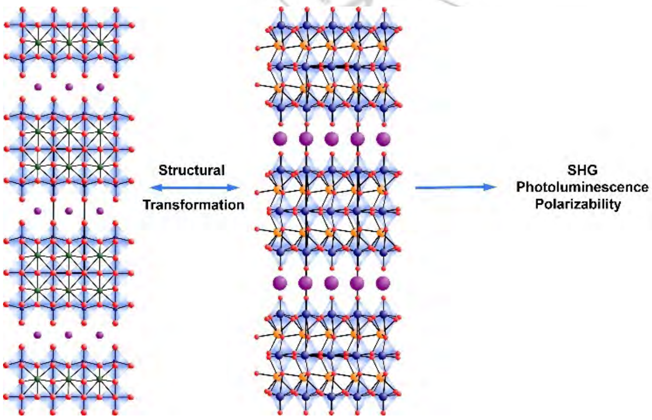
Event Hall FRI 11:00~13:00

Solid-State Syntheses and Optical Properties of Eu^{3+} -Doped *n* = 3 Layered Perovskite Solid-Solutions

Jin kyu Kim, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Pure polycrystalline materials of *n* = 3 layered Dion-Jacobson (DJ) perovskites have successfully synthesized through conventional solid-state reactions. Structures for the noncentrosymmetric phase and centrosymmetric phase were refined in the space group, *Ima*2 and *P*4/*mmm* respectively, by the Rietveld method using the powder X-ray diffraction. Because the symmetry for the *n* = 3 layered DJ perovskite is strongly influenced by the occupation of Bi^{3+} and Eu^{3+} cations, the diffraction patterns were carefully analyzed as we change the Eu^{3+} -doping ratio on the A site of the materials. Second harmonic generation (SHG) and photoluminescence (PL) properties of the layered perovskites have been carefully studied by changing the amount of doped- Eu^{3+} cations. The origins of the observed SHG and PL properties for the reported materials are also elucidated.



Poster Presentation : **INOR.P-131**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

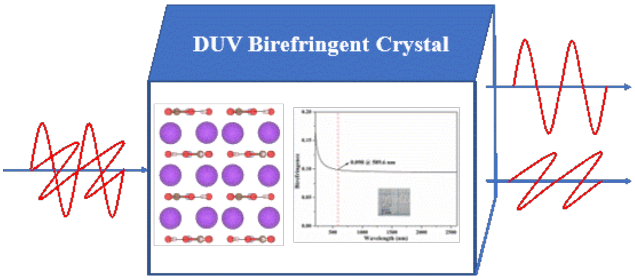
A promising birefringent crystal in the deep ultraviolet region

Yang Li, Kang Min Ok[1,*]

Chemistry, Sogang University, China

[1]*Department of Chemistry, Sogang University, Korea*

Birefringence is one of the key paraments to the birefringence materials, also very important to the SHG materials. The commercially applied birefringent materials could apply in different wavelengths from Deep Ultraviolet (DUV) to Near-Infrared (NIR) regions. The optimal arrangement π-conjunction groups (B_3O_6, BO_3, etc.) and the d^{10} octahedra are beneficial to design compounds with large birefringence. Among the organic groups, analogous to the B_3O_6, $C_3N_3O_3$ possess even larger microscopic polarizability anisotropy. Besides, cations with SCALPEs also could strongly enhance the birefringence, too. In the DUV region, MgF_2 and α-BaB_2O_4 (α-BBO) are could not meet all the rigid requirements, such as the quite small birefringence of MgF_2 and the phase-transition, cracking problem of α-BBO. Previous work points out introduce hydrogen into coplanar can enhance the bandgap and the birefringence.[1] In addition, combine with F, the compounds should further blueshift the UV cutoff edge. Consideration of the above ideas, via the facile aqua-solution method, transmittance crystal size up to 7□6□2 mm^3 is obtained. The UV cut-off edge (smaller than 200 nm), the considerable birefringence (0.098 @ 589.6 nm), and the facile growth method point out it is a promising birefringent crystal that could be applied in the DUV region.[1] W. Cai, J. Chen, S. Pan, Z. Yang, Enhancement of Band Gap and Birefringence Induced via π-Conjugated Chromophore with "Tail Effect," Inorg.Chem.Front.(2021). https://doi.org/10.1039/d1qi01270c.Keywords: Birefringent Crystal; Birefringence; DUV Region.



Poster Presentation : **INOR.P-132**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Investigation of ammonia adsorption capacity in MIL-101/reduce graphene oxide under high pressure

Cheongwon Bae, Mingyu Gu, Yeram Kim, Juyeong Kim*

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Korea

Carbon-free energy applications have been actively developed to deviate fossil fuel-based systems. An Adsorption heat pump emerges as an alternative to conventional heating and cooling systems by applying efficient working fluid-adsorbent pairs as well as waste heat. Herein, we developed a nanocomposite with MIL-101-NH_2 (MIL-A) and reduced graphene oxide (rGO) via a one-pot hydrothermal reaction. The sheet-like nanocomposite seemed to retain unique pore structures with mesoscale cavities between rGO and MIL-A nanoparticles. We supposed that such pore structure could improve the working capacity for high-pressure ammonia adsorption and desorption. Our nanocomposite displayed higher ammonia adsorption capacity at 5 bar than each single component. Our strategy to incorporate rGO into MIL-A will also be applicable to other metal-organic frameworks for enhancing high-pressure ammonia uptake.

Poster Presentation : **INOR.P-133**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Lattice-Guided Construction of a Naturally Nonpreferred Metal-Organic Framework

Sujeong Lee, Gihyun Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The components and structures of materials are critical two elements, which determine MOFs' properties and so applications. During the MOF construction, best components with ideal functionalities or characteristics are relatively easy to access by an appropriate choice from many existing chemical libraries or by designing new ones. However, the construction of MOFs with a desired structure is rather challenging. Typically, nature decides a MOF structure to have thermodynamically and/or kinetically favoured one within the supplied components. Herein, we report an advanced approach for the concurrent designation of both components and structure of a MOF during its construction.

Poster Presentation : **INOR.P-134**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Rational Manufacture of Yolk–Shell and Core–Shell Metal Oxide Double Layers from Coordination Polymer Double Layers

Gihyun Lee, Sujeong Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

Metal oxides with various metal compositions have received huge attention due to their useful applications in magnetics, optics, catalysis, and sensing. In addition, the manufacture of well-designed yolk–shell materials is great concerns in material development due to the many benefits derived from the structural features. Herein, we report an easy method for the selective manufacture of yolk–shell or core–shell-type hybrid metal oxide double layers (silica@MxOy@M'x'Oy'; M and M' = Er, Y, Tb, or Gd) via thermal treatment of the silica-templated coordination polymer (CP) double layers (silica@MCP@M'CP), which are prepared via two-step CP growth on the carboxylic acid-terminated silica microspheres. The production of a yolk–shell or core–shell structure from the silica@MCP@M'CP is found to be regulated by the thermal decomposition properties of the two CP layers within silica@MCP@M'CP. One-step decomposition of the two CP layers results in a core–shell metal oxide double layer, whereas two-step sequential decomposition of the two CP layers with time interval between the first and second decompositions results in a yolk–shell metal oxide double layer.

Poster Presentation : **INOR.P-135**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Spectroscopic Evidence for a Peroxyhemiacetal-Like Intermediate in Nucleophilic Reaction

Yeongjin Son, Jaeheung Cho[1,*]

Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Chemistry, UNIST, Korea*

In the biological system, metal-bound peroxyhemiacetal species have been proposed to be key intermediates in aldehyde deformylation reactions by nucleophilic attack of metal-peroxo complexes.[1] However, there is still considerable debate on the initial step in the aldehyde deformylation.[2-4] Herein, we report the first spectroscopic characterization for a mononuclear cobalt(III)-peroxyhemiacetal complex, [Co(Me3-TPADP)(O2CH(O)CH(CH3)C6H5)]+ (2, Me3-TPADP = 3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane), in the reaction of a cobalt(III)-peroxo species (1) with 2-phenylpropionaldehyde (2-PPA), which was characterized by various physicochemical methods such as UV-vis, CSI-MS, IRPD, EPR, 1H NMR. Isotope labeling experiments showed that the carbonyl group of 2-PPA inserts between the oxygen atoms of 1 in the initial step of the aldehyde deformylation reaction. The equilibrium between 1 and 2 was identified with a small equilibrium constant. In the presence of an excess amount of 2-PPA, 2 decomposed to give cobalt(II) species and deformylated products. The reaction of 1 with other aldehydes also showed the formation of a peroxyhemiacetal species. The investigation of the peroxyhemiacetal intermediate provides significant insight into the initial step of aldehyde deformylation by metalloenzymes.

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April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-136**

Inorganic Chemistry

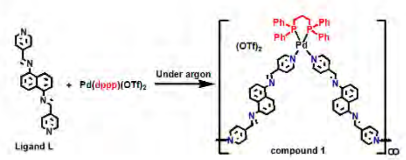
Event Hall FRI 11:00~13:00

A 1D Palladium coordination polymer and its catalytic activity in Suzuki coupling reaction

Gang Min Lee

Department of Chemistry, Sungkyunkwan University, Korea

Our research group has been interested in the design of linking ligands, as well as the preparation of their coordination polymers. Herein, we report the crystal structure of a 1D Palladium coordination polymer and its catalytic activity in the Suzuki coupling reaction.



Poster Presentation : **INOR.P-137**

Inorganic Chemistry

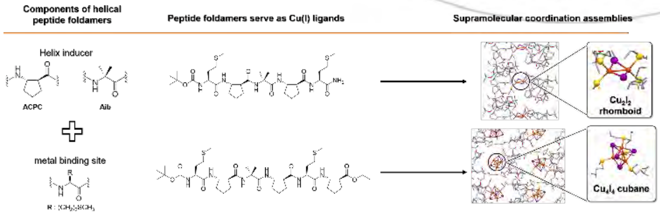
Event Hall FRI 11:00~13:00

Constructing Supramolecular Coordination Assemblies with Helical Peptide Foldamers

Jaewook Kim, **Hee-Seung Lee***

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

2-Aminocyclopentanecarboxylic acid(ACPC) and 2-aminoisobutyric acid (Aib) are well-known for inducing helical structures of short peptide foldamers. Their folding propensity makes them attractive templates for numerous supramolecular assemblies. This made us conceive an idea of controlling supramolecular coordination assemblies with the help of pre-organized foldamer ligands. From this vision, we synthesized two types of ACPC/Aib-contained peptide foldamers that two methionines, which act as metal-binding sites, are introduced in the sequence. Coordinating these foldamers with copper(I)-iodide formed micro-sized crystals containing Cu_2I_2 rhomboid or Cu_4I_4 cubane clusters depending on the sequence length of the peptide foldamer. We also found Cu_4I_4 cubane clusters are connected in an extended coordination network and form open frameworks. While these coordination assemblies are promising multifunctional platform materials with inherent chirality, we cannot wait to reveal their potential for technological applications.



Poster Presentation : **INOR.P-138**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Full-Wavelength Photoconversion of CO2 by Colloidal Nanocatalysts

Byeonghoon Choi, Hyunjoon Song[1,*]

Korea Advanced Institute of Science and Technology, Korea

[1] *Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Generating alternative energy from greenhouse gases is a promising environmental technology. Semiconductor photocatalysts have been intensively studied due to their great potential for treating solar energy. We focused on photoreduction of CO2 into value-added compounds such as methane or carbon monoxide. To overcome charge recombination and improve catalytic performance, we focused on heterojunction compounds. We synthesized ZnO@Cu2O, hollow TiO2@Cu2O and g-C3N4@Cu2O nanostructures. These photocatalysts exhibit high photocatalytic activities and selectivities under full-wavelength irradiation. Furthermore, for utilizing more solar energy, we propose to expand our research area to visible light-responsive photocatalysis.

Poster Presentation : **INOR.P-139**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

One-Pot Synthesis of Palladium Organometallic Frameworks with Carboxylic Acid Directed C-H Activation

Jong-Yeong Jung, Hyunjoon Song*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Metal-Organic Frameworks (MOFs) have received attention over the past two decades for their structural diversity and tunability based on coordination chemistry. Recently, research to diversify not only metal elements but also the elements bonded to metals into elements other than oxygen or nitrogen is being conducted, and traditional organometallic chemistry has emerged to contribute to the new flow. Herein, we one-pot synthesized a palladium organometallic framework, PdOF-1, by introducing a conventional catalytic reaction, palladium-catalyzed *ortho* C-H activation. Atomically dispersed palladium atoms are the only metallic element in this framework, and labile Pd-C bonds constitute the two-dimensional network. The organometallic framework (OMF) shows a solid-to-solid phase transformation by post-synthetic thermal activation due to its lability. This work proposes a strategy to synthesize noble metal networks without aggregations to noble metal nanoparticles and construct OMFs with M-C bonds.

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April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-140**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Correlation between Metal-ligand Interaction and Electrochemical H_2 Evolution Reaction

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[1]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

First-transition metal complexes are widely studied to provide alternatives of noble metal catalysts, such as Pt, Re, and Ir. The first-transition metal complexes have shown high catalytic performances in electrochemical reduction reactions. Among these metal complexes, pincer complexes are spotlighted for their high catalytic performance through facile structural modifications. We investigated metal-ligand interactions using NNN-pincer complexes containing various auxiliary ligands and metal ions. Our NNN-pincer complexes showed different electrochemical properties depending on auxiliary ligands such as polypyridyl and isocyanide ligands. Additionally, the secondary-coordination sphere at NNN-pincer ligand affected the catalytic performance by stabilizing the reaction intermediates. In this poster, we will discuss the electrochemical data of the synthesized NNN-pincer complexes and the current understandings of the reaction mechanisms with DFT calculation results.

Poster Presentation : **INOR.P-141**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

$M(II)AlF_5{\cdot}7H_2O$ (M = Fe, Co, and Ni): Synthesis, Structure, and Characterization of New Mixed Metal Fluoride Hydrates.

Sun Woo Kim

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Three new mixed metal fluorides hydrates, $M(II)AlF_5{\cdot}7H_2O$ (M = Fe, Co, and Ni) were synthesized and characterized. Crystals of $M(II)AlF_5{\cdot}7H_2O$ were obtained by hydrothermal method using CF_3COOH aqueous solution. $M(II)AlF_5{\cdot}7H_2O$ crystallizes in both *C*2/m (No. 12) or *P*-1 (No. 2) space groups depending on the temperature. The phase transition of $M(II)AlF_5{\cdot}7H_2O$ is attributable to the change of the bonding environment of $[M(II)(H_2O)_6]^{2+}$ and $[Al(III)F_5(H_2O)]^{2-}$ octahedra according to the temperature change. FT-IR and TGA analysis of $M(II)AlF_5{\cdot}7H_2O$ confirmed the presence of water molecules. UV-Vis spectra of $M(II)AlF_5{\cdot}7H_2O$ showed unique absorption band depending on the $[M(II)(H_2O)_6]^{2+}$ cation. Detailed synthetic procedure, crystal structure, and characterization of $M(II)AlF_5{\cdot}7H_2O$ will be presented.

Poster Presentation : **INOR.P-142**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

2D-Confined Reduction of Nickel Hydroxide towards Thermally Stable Ultrasmall Nanocatalysts for Stable Dry Reforming of Methane

Sunwoo Jang, In Su Lee[1,*]

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Quest for green energy solutions and CO2 remediation is driving the urgent demand for advanced catalytic platforms. As a major bottleneck: under high temperature operation, conventionally supported catalytic nanocrystals (NCs) undergo sintering and deactivation which is highly challenging to control. Here, we introduce lamellar confinement strategy for ‘sheet-to-NCs’ conversion within a 2D-silica envelope, which constructs a catalytic nano-cartridge holding a platoon of isolated and in-plane-aligned ultrasmall NCs (Ni-SiCart), performing as robust and coking-resistant catalytic system for dry reforming of methane. Overcoming the problem of unavoidable bulk phase growth from multiple sheet-stacks or single sheet-on-open-support, 2D-silica conformal bilayer-encasing tightly clamps the atomically thin Ni(OH)2-sheet during thermal metallic conversion and further hinders the in/out-of-plane migratory fusion of the resultant Ni NCs. Upon heating-cooling cycle, the plastically deformable glassy-phase endows flapping of silica envelope, which clutches the Ni NCs like ‘eggs in a carton’, subsequently, ensuring their thermal stability. Owing to the unique 2D-enveloped rigid architecture, Ni-SiCart can circumvent sintering and coke deposition while tolerating the high temperatures (>700 °C) for long operation (>100 h), affording high conversions to syngas.

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Poster Presentation : **INOR.P-143**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Status of BL2D supramolecular crystallography beamline at Pohang Light Source II

Dae-Woong Kim, Dohyun Moon*

Beam Operation Team, Pohang Accelerator Laboratory, Korea

Supramolecular Crystallography Beamline (BL2D-SMC) at the Pohang Accelerator Laboratory is the only crystallography laboratory facility in Korea using synchrotron radiation accelerator and is a device for analyzing small molecule and supra molecule structure. Structural analysis using various experimental devices such as using a short wavelength of 1.2 ~ 0.6 Å, 90K ~ 450K temperature and gas adsorption is possible and these devices can be easily used by users through beamline software (BL2D-SMCD). BL2D is performing not only general single crystal data collection such as hollow molecular structure (MOFs, cage structure, and very tiny size crystal (< 10 µm3)) but also non-ambient crystallography with variable temperature, gas sorption and photo-excitation to the crystal. The instruments, status and diverse application using BL2D will be introduced in this presentation.

Poster Presentation : **INOR.P-144**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Air and oxygen stable perovskite nanocrystal for LED application

Yongju Hong, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The visualization of accurate color information using metal halide perovskites has been explored recently with a great fervor, because of their superior optical properties such as high photoluminescence quantum yield (PLQY), excellent color purity, and facile bandgap tunability. The achievement of white light and accurate color renderings in real-world applications require the development of efficient and stable perovskite light-emitting diodes overcoming their inherent instability. The cesium lead mixed-halide perovskite nanocrystal (PNC) system in the form of a well-tailored core/shell structure with a semiconductor shell offers a pathway towards highly stable perovskite-based displays. However, it remains challenging to access the epitaxially well-tailored core/shell architecture because of the limited methodology. Here, we present a systematic strategy of preparing uniform perovskite core with epitaxially grown semiconductor shell. We found that post-synthetic treatment is effectively passivating surfaces by defect elimination in the crystalline structure, thereby facilitating the epitaxial growing of the shell and significantly improving the intrinsic stability with high luminescence efficiency. We constructed the perovskite-based light-emitting diodes (LEDs) that exhibit superior external quantum efficiency (EQE) and luminance, representing a performance superior to that of state-of-the-art blue perovskite-LEDs. We anticipate that our core/shell perovskite blue light-emitting devices can greatly facilitate the development of electroluminescent full-color displays using perovskites.

Poster Presentation : **INOR.P-145**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Photoluminescent two-dimensional polymers of zinc(II) and copper(I) ions including pyridine-based ligands

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[1]*Department of Chemistry Education, Kyungpook National University, Korea*

Two-dimensional (2-D) coordination polymers [Zn2(bpab)(CH3CO2)4]•H2O (1), [Zn(bpab)(H2O)2](NO3)2 (2), [Cu2(bpab)I2]•CH3OH (3), and [Cu2(tpmd)I2] (4) have been synthesized by the reaction of zinc(II)/copper(I) ions and tetradentate polypyridine ligands (bpab = bis-1,4-(di-4-pyridylaminomethyl)benzene and tpmd = N,N,N',N'-tetrakis(pyridine-4-yl)methanediamine). The zinc(II) ions of 1 and 2 have distorted tetrahedral and trigonal bipyramidal geometries, respectively. By coordinating zinc(II) ions and bpab ligands, 1 and 2 formed a brick wall and puckered 2-D networks, respectively. The copper(I) ions of 3 and 4 are both tetrahedral structures with Cu2I2 rhomboidal geometry. By linking the Cu2I2 cores and bpab/tpmd ligands, 3 and 4 exhibited interwoven and interconnected bilayered 2-D networks, respectively. Compared to free bpab and tpmd ligands, polymers 1 and 2 show strongly blue-shifted emissions, whereas polymers 3 and 4 show strongly red-shifted emissions. Therefore, the shifts of emission wavelengths are strongly dependent on the zinc(II) and copper(I) ions that linked the bpab/tpmd tetradentate ligands, respectively. In this poster, we will present and discuss the synthesis, structure, and physical properties of 1-4.

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Poster Presentation : **INOR.P-146**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Electrocatalytic H_2 Evolution by Cobalt Complexes

<u>JuEun Lee</u>, Junhyeok Seo*

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Dihydrogen is a promising future energy carrier, and electrochemical hydrogen evolution reaction (HER) would be a sustainable method to generate the gas. For this, intensive research efforts are focused to develop the electrochemical hydrogen evolution reaction (HER) catalysts. Among various catalyst designs, recent reports have shown that a redox-active ligand could enhance the catalytic activity of HER catalysts by lowering the overpotential. Herein, we utilized bipyridine(bpy)-conjugated Co complexes to study the HER reactions. We examined the Co-bpy system by extending the pi-conjugation with an imine moiety. The modified bpy-imine moiety significantly enhanced the HER catalytic activity by lowering the overpotential. The cobalt complexes show several catalytic pathways varied by pka of proton sources, and we try to follow the reaction mechanism with DFT calculations. In this poster, we will discuss the electrochemical behaviors of the Co-bpy complexes and the current understandings of the reaction mechanisms.

Poster Presentation : **INOR.P-147**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Electrochemical CO_2 Reduction by pincer-type Co Complexes

Wonjung Lee, Seungjin Song[1], Junhyeok Seo[*]

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

[1]*Chemistry, Gwangju Institute of Science and Technology, Korea*

Gaseous CO_2 can be a carbon source for producing the value-added carbon products. Electrochemical CO_2 reduction is a simple pathway for CO_2 transformation, but the poor selectivity and low efficiency remain challenges because of another competitive reaction - proton reduction. For decades, researchers have tried to develop electrocatalysts at molecular levels and particularly, could enhance catalysts in terms of the reactivity and selectivity by introducing π-conjugated ligands. Recently, polypyridyl complexes have obtained research interests due to the excellent ability to stabilize transition metal ions during the elctrochemistry as well as to enhance the electrochemical CO_2 reduction. Herein, we examined polypyridyl complexes, especially as coordinated together with NNN-pincer-type ligands. We could observe the enhanced CO_2 reduction reactivity with the appropriate combination of a polypyridyl and an NNN-donor set. In this poster, we will discuss the CO_2 reactivity of Co complexes and the reaction mechanism.

Poster Presentation : **INOR.P-148**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Blue TADF Emitters Incorporating *B*-Heterotriangulene Acceptors for High-Efficiency OLEDs with Suppressed Roll-Off

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Department of Chemistry & Chemical Industry Research Institution, University of Ulsan, Korea
[1]*Department of Chemistry, University of Ulsan, Korea*

We report a family of boron-based rigid blue TADF emitters (**1—3**) incorporating 9,9-dimethyl-9,10-dihydroacridine (DMAC) donor and triply-bridged *B*-heterotriangluene acceptors tethered by three methylene bridges (**1** and **2**) or two methylene and one oxygen-bridges (**3**) for blue organic light-emitting diodes OLEDs. The X-ray crystal structures of **2** and **3** exhibited a highly twisted molecular geometry between the donor and acceptor units, and a completely planar structure for the *B*-heterotriangulene fragment. The doped host films of all compounds displayed blue emissions with the unitary PLQYs, small singlet-triplet energy splitting (< 0.1 eV), fast reverse intersystem crossing rates ($k_{\mathrm{RISC}} \sim 10^6$ s^{-1}), and short-lived delayed fluorescence ($\tau_d \sim 2$ μs). Using these compounds as the emitters, we realized highly efficient blue TADF-OLED devices. In particular, the fully methylene-bridged emitter (**2**) showed the highest external quantum efficiency (EQE) of 28% and the lowest efficiency roll-off, maintaining a high EQE value of 21% at 1000 cd/m^2.

Poster Presentation : **INOR.P-149**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

AgxCd1-0.5xS Decorated Cadmium Sulfide Nanowires with Exceptional Selectivity in Photocatalytic Conversion of Benzyl Alcohol

Seojin An, Hyun Sung Kim[*], Joo Hyun Kim[1]

Department of Chemistry, Pukyong National University, Korea
[1]*Department of Polymer Engineering, Pukyong National University, Korea*

We here demonstrate the controlled synthesis of Cadmium Sulfide nanowires (CdS NWs) decorated AgxCd1-0.5xS via simple Ag+ ion exchange method. The AgxCd1-0.5xS are deposited on the surface of CdS NWs, forming a heterogeneous interface of AgxCd1-0.5xS and CdS NWs (002) planes, which promotes the separation efficiency of photogenerated charges and improves the catalytic performance in photoconversion from benzyl alcohol to benzaldehyde or C-C coupling products. Importantly, the product of the photocatalytic reaction varies depending on the amount of x in AgxCd1-0.5xS. When x is greater than 0.2, the main product is C-C coupling, and when x is less than 0.2, the main product is benzaldehyde, showing a specific selectivity. The in-situ HR-XPS results corroborate the superior selectivity of AgxCd1-0.5xS / CdS NWs is mainly due to the formation of a built-in electric field and dependence on whether AgxCd1-0.5xS as a cocatalyst accepts an excited electron or a hole in CdS NWs. In all, this study reports a simple in-situ hydrothermal growth protocol to efficiently construct AgxCd1-0.5xS / CdS NWs heterojunction composites and offers guidelines for design of a new synthetic strategy to prepare efficient photocatalysts.

Poster Presentation : **INOR.P-150**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Porphyrin crosslinked PVA nanofiber for photocatalytic degradation of 2-CEES, a chemical warfare agent simulant.

Juno Hyeon, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

Chemical warfare agents (CWAs), including Tabun (GA), Sarin (GB), Soman (GD) and VX, have been threatening to life and environment for decades. Great research efforts have been focused to reduce the world-wide stockpiles of CWAs. The current state-of-art techniques include combustion, pyrolysis, hydrolysis and photocatalysis. Among them, photocatalysis has become one of the most extensively studied field for the destruction of CWAs. Herein, we like to demonstrate fiber type of photocatalyst. Electrospinning was conducted to fabricate photocatalytic nanofiber. Porphyrin was selected as an active photocatalyst and was successfully dispersed in the nanofibers. Moreover, the porphyrin crosslinked polymers to enhance the stability when nanofiber formed. Consequently, photocatalytic activity toward 2-CEES, simulant of a mustard gas that causes blisters on the human skin, was performed under blue light irradiation. Furthermore, the stability of the materials was testified under various solvents and the sustainability test were performed for potentially applicable to the real field as masks or suits against chemical threats.

Poster Presentation : **INOR.P-151**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Boron-Carbonyl Hybrid Acceptors Having Modified Electronic Conjugation for Efficient Orange-to-Red TADF Emitters

Ina Nur Istiqomah, Taehwan Lee*, Hanif Mubarok*, Ju Hyeong Kim*, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

The development of high-performance orange-to-red organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) emitters still remains a great challenge to achieve full-color display applications. In this study, we designed and synthesized a series of donor (D)–acceptor (A)-type orange-to-red TADF emitters, namely PXZBAO (**1**), PXZBTO (**2**), and PXZBPO (**3**) comprising conjugated planarized boron-carbonyl hybrid acceptors and a phenoxazine donor. The compounds exhibited emissions in the orange-to-red region (λ_{PL} = 619–574 nm) in toluene solution. In particular, the emission wavelength was blue-shifted with the increase of the number of the benzene rings in the boron acceptors. All compounds have small singlet-triplet energy splitting ($\Delta E_{ST} < 0.1$ eV), very short-lived delayed fluorescence lifetime ($\tau_d < 2$ μs), and high k_{RISC} of ca. 10^6 s^{-1}, which supported the strong and efficient TADF properties. The details of synthesis, characterization, and photophysical properties will be discussed.

Poster Presentation : **INOR.P-152**

Inorganic Chemistry

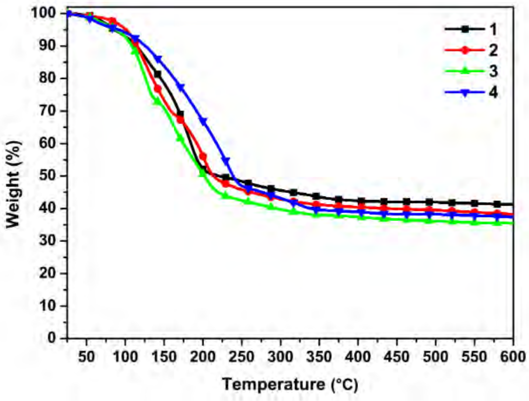
Event Hall FRI 11:00~13:00

Synthesis of Highly Volatile Indium Precursor with Oxygen-Free Cyclic Amine Ligands

Ji-seoung Jeong, Bo Keun Park, Ji Yeon Ryu*

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea

A series of iminopyrrolidinate indium complexes with high volatility was synthesized to use as a precursor for the fabrication of nanoscale thin films. All complexes 1 - 4 were fully characterized by multinuclear NMR, IR, elemental analysis, mass spectroscopy, X-ray crystallography as well as thermogravimetric analysis. These complexes showed different chemical/physical properties depending on saturated cyclic ring and the presence of an alkyl group. The solid-state structure of 1 revealed dimeric structure which consists of the two cyclic amine ligands bridges between the two indium metals. Interestedly, complexes 2 – 4 are monomer conformers and exist as a liquid at room temperature. Furthermore, multinuclear NMR and mass spectra clearly indicated the monomer formation. Thermogravimetric analysis (TGA) showed that all complexes weight loss before reaching 100°C. Complexes 1 and 4 showed a mass loss pattern of 2 steps, and residual masses of 39% and 36% were observed, respectively. Also, complexes 2 and 3 showed a mass loss pattern of 3 steps, and residual masses of 37% and 35% were observed, respectively.



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Poster Presentation : **INOR.P-153**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Tunable Hollow Silica Nanostructures and their Ordered Mesoscale Assembly

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[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Despite the enormous applications and fundamental scientific interest, synthesis of amorphous hollow-silica nanostructures in crystal-like non-spherical polygonal architectures is challenging. Herein, we present a facile one-shot synthetic procedure for various unconventional hollow-silica with controllable surface structures by addition of a metal salt and implementing kinetic handles of silica precursor (silanes/ammonia) concentrations and reverse-micellar volume. During the silica growth, we identified the key role of metal coordination complexes as a nano-polyhedral temporary template, which provides the facet-selective interactions with amino-silica monomers and guides the differential silica growth that produce different structures. Additionally, the crystal-like polygonal hollow-silica with flat surfaces, assembled as highly ordered close-packed octahedral mesoscale materials (ca. 3 μm) where hollow-silica act as building-units (ca. 150 nm) to construct cavities and nanospaces.

Poster Presentation : **INOR.P-154**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Fabrication of PdAgPt Nanosheets by controlling the composition for enhanced alcohol oxidation reaction

JiEun Yu, Jong Wook Hong*

Chemistry, University of Ulsan, Korea

The functions of heterogeneous nanocrystals will be doubtless tuned by controlling their morphologies and compositions, beside that it is challenging to fabricate the nanoparticles that have superior activity and stability for fuel cell reaction. Alloying metals and controlling the morphology are promising way to increase electrocatalytic activity and stability of nanoparticles, which modify the electronic structure of nanoparticles. Herein, we synthesized PdAgPt trimetallic nanosheets for Ethanol Oxidation Reaction by controlling molar ratio of metal precursors. The electronic structure of nanosheets can be changed by incorporation of the elements and undercoordinated atoms that exist at the edge site of nanosheets. Therefore, PdAgPt Nanosheets have higher mass and specific activity with 10442 mA mg-1 and 27.4 mA cm-2 in ethanol oxidation reaction compared with commercial Pd or Pt catalysts.Keywords: two-dimensional, ethanol oxidation, trimetallic, dendritic, electrocatalysis

Poster Presentation : **INOR.P-155**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

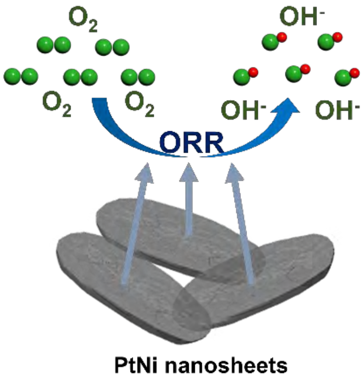
2D Ultrathin PtNi Porous Nanosheets for Highly Active Oxygen Reduction Electrocatalysis

Pramadewandaru Respati Kevin, Jong Wook Hong*

Chemistry, University of Ulsan, Korea

Platinum-based 2D ultrathin porous nanosheets catalyst have great potential to solve the problems of highly active catalyst for oxygen reduction reaction (ORR) within proton exchange membrane fuel cells (PEMFCs). Herein, the Pt-Ni nanosheets catalyst with different atomic ratio were developed by a synthetic strategy of alloying process of nickel into platinum nanosheets (Pt NSs) produce the unique porous sheets structure from the oxidation etching process. The ORR electrocatalytic performance of various PtNi NSs were investigated using pristine Pt Ns and commercial Pt/C catalyst for comparisons. It is found that the Pt3Ni NSs catalyst have the optimum ratio showed excellent ORR performance. At 0.9 V vs. RHE, Pt3Ni NSs achieved higher mass activity (MA) 2.27 A mg-1Pt and specific activity (SA) 4.71 mA cm-2Pt compared to pristine Pt NSs (0.45 A mg-1Pt & 0.85 mA cm-2Pt)and commercial Pt/C (0.23 A mg-1Pt & 0.39 mA cm-2Pt) catalyst. Superior performance of Pt3Ni NSs was mainly attributed to: i) The ultrathin layer structure, ii) alloying with transition metal, iii) high porous sheets at the edge sites of nanosheets.

Keywords: Pt-based nanocatalyst, Pt-Ni alloy, ultrahin porous nanosheet, oxygen reduction reaction.



Poster Presentation : **INOR.P-156**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Palladium-Lead Nanobranches Electrocatalysts for Ethanol Oxidation Reaction in Alkaline Medium

Dian Tri Lestarini, Jong Wook Hong*

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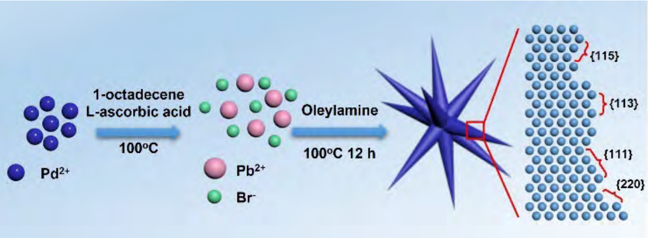
Bimetallic nanocrystals (NCs) with controlled uniformity of morphology and composition endow a great ability in modifying the electronic properties and possess the synergistic effect to enhance their electrocatalytic performance. Combining Pd with Pb can improve the poisoning tolerance of Pd during electrocatalytic reaction. Pb can provide abundant oxygen-containing species (OH_{ads}) and the ability to cleavage C-C bond during electrocatalysis that can hinder the production of CO_{ads} species thereby improving the ethanol oxidation reaction (EOR) performance. Herein, we report a highly uniform branch of Pd_3Pb NCs has been prepared via a wet-chemical approach. The growth process of Pd_3Pb Nanobranches (NBs) was controlled by ascorbic acid as a reductant, oleylamine (OAm), and 1-octadecene (ODE) as a solvent and surfactant, and ammonium bromide (NH_4Br) as a shape-directing agent. The unique morphology of Pd_3Pb NBs is suitable as electrocatalysts due to expose high-index facet which possesses high specific surface area, and a high density of under-coordinated surface atoms that can enhance EOR in alkaline media. The results confirm that Pd_3Pb NBs exhibited much higher mass activity (5231 mA mg^{-1}) compared to Pd_3Pb nanocubes (3522 mA mg^{-1}) and commercial Pd/C (1636 mA mg^{-1}). This work presents a new design of nanoparticles structure by modifying the morphology and composition for highly active and durable catalysts for fuel cells and beyond.



Poster Presentation : **INOR.P-157**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Transformation of Alkyl Azide to Valuable compounds with Co-Si pincer complexes through Metal-Ligand Cooperation

Yunho Lee*, **Kunwoo Lee**[1]

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[1]*Chemistry, Seoul National University, Korea*

Isocyanate is an important material for synthesis of polyurethane which is used as flexible and rigid foam, fibers, etc. But the industrial synthetic method of it still uses highly toxic phosgene. Our research team tried to develop the method to produce isocyanate with imitation of CODH activation site by methyl SiP2 tridentate pincer ligand through metal-ligand cooperation. In 2021, we succeeded in transferring the nitrene group using a MeSiP2 (MeSiP2 = MeSi[2-Pi Pr2-C6H4]2)-Cobalt complex and 365nm UV radiation. However, this transformation has low efficiency(TON is 5 in optimized condition). To improve the capability as a catalyst, we changed the substituted part of the Si center to Ph and computationally calculated it. The result showed a positively 2.15kcal/mol lower activation energy expectation than the methyl version. Since methyl substituted one was conducted under CO atmosphere, it’s only done without CO condition and shows 4.3 turnover for the same condition. Nevertheless, we can reuse 20% of it by adding CO after the reaction unlike the previous catalyst. Now, we’re working to the optimization the reaction and apply for other useful synthesis such as aziridination or oxyazetidination.

Poster Presentation : **INOR.P-158**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Optimal size of nanorods in metal-semiconductor nanostructures for efficient photocatalytic hydrogen generation and kinetic modeling

Bumjin Park, Hyunjoon Song*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Metal chalcogenides-based nanostructures have been suggested as attractive materials for efficient photocatalysts under visible light irradiation. Herein, we synthesized different lengths of CdSe nanorods and Pt tipped nanorod structures to demonstrate the correlation between reactivity and the distance of electron acceptors. We revealed that the hydrogen-evolution rate was directly proportional to the amount of long-lived charge-transfer state dominated by the carrier diffusion to the metal center. As the nanorod length increased, the carrier-diffusion rate decreased, while the absorption cross-section increased. As a result, the number of carriers migrating to the metal tips was the optimum at the 15-20 nm nanorods per tip, in good agreement with our hydrogen-evolution experiments. This information provides a direct guideline to design the optimal geometrical configuration of metal–semiconductor hybrid nanocatalysts.Keywords: Hybrid nanorod, Photocatalyst, Hydrogen evolution, Charge transfer, Transient absorption spectroscopy

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Poster Presentation : **INOR.P-159**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Adsorption of Mn using iron oxides and mitigation of Mn toxicity in soil contaminated with chromium.

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Department of Agricultural Chemistry, Chungbuk Natioanl University, Korea
[1]*Environmental and Biological Chemistry, Chungbuk National University, Korea*

Manganese exists in various oxidation states in soil, Mn(II) is most mobile form among Mn species. Contamination of soil with Cr(III) increased bioavailable Mn concentration in soil, which was toxic to plants. Therefore, the objective of the study was to reduce manganese toxicity in soil. Iron oxides such as ferrihydrite, schwertmannite, hematite, and goethite were selected as adsorbent for Mn. In order to evaluate Mn(II) immobilization by iron oxide, 0.2 g of iron oxide was reacted with 25 mL of Mn(II) solution. After the reaction, the Mn concentration was analyzed using an inductively coupled plasma atomic emission spectrometer. Solid phase Mn was analyzed using X-ray absorption spectroscopy and X-ray diffraction. Although mineralogy of Mn was not changed after Mn adsorption, Mn was oxidized in the order of ferrihydrite, goethite, hematite, and schwertmannite. CaCO3, CaNO3, CaSO4 and organic matter were treated to alleviate Mn toxicity in Cr(III) spiked soils. CaCO3 and CaNO3 reduced bioavailable Mn concentration and can be applied in the soil to mitigate Mn toxicity in Cr(III) contaminated soil without affecting Cr toxicity.

Poster Presentation : **INOR.P-160**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Mechanistic Dichotomy in Sulfoxidation with an Iron(III)-Hydroperoxo Complex Derived from Proton- and Salicylate-Assisted Dioxygen Activation

Hyeri Jeon, Hyungbin Park, Seungwoo Hong*, Chaewon Ahn

Department of Chemistry, Sookmyung Women's University, Korea

During past decades, synthetic mononuclear nonheme iron-oxygen species such as iron-superoxo, -peroxo, -hydroperoxo, and -oxo intermediates have been extensively scrutinized by means of various spectroscopic techniques in order to discern the nature's way of perplexing oxidative transformations. Also, there is a growing interest in exploiting biomimetic metal complexes as a route to ultimately build up and develop novel catalysts. Among progress done in this field, iron(III)-hydroperoxo intermediates have recently been attracted much attention due to its intrinsic amphoteric reactivity; both electrophilic and nucleophilic reactivity have been assessed without cleaving the O–O bond (i.e., the involvement of iron(IV or V)-oxo intermediates). Herein, we report the synthesis and characterization of the iron(III)-hydroperoxo complex originated from the salicylate-assisted dioxygen activation by iron(II) complex bearing cationic ligand. Combined spectroscopic and theoretical data suggested that end-on hydroperoxo ligand was coordinated to the iron center and stabilized due to the presence of cationic ligand. Interestingly, mechanistic dichotomy was confirmed by reacting para-substituted thioanisoles and plotting their kinetic data in hammett plot.

Poster Presentation : **INOR.P-161**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Two-dimensional $Cu_{2-x}S/CdS$ heterostructured nanoplates via a cation exchange for visible-light-driven photocatalytic hydrogen generation

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Quantum confined semiconductor nanomaterials have been attracted for promising photocatalysts which can convert solar light to chemical energy. Among the various reactions, hydrogen evolution from photocatalytic water splitting is valuable. For higher photocatalytic hydrogen generation efficiency, heterostructured photocatalysts are necessary for prohibiting charge recombination and increasing charge separation. Metal sulfides are well-known materials for improving water-splitting reactions because they can utilize visible light. Moreover, two-dimensional semiconductor nanostructures have the advantage of larger surface area, more exposed active sites, and charge transfer than one-dimensional structures for photocatalyst. Herein, we synthesized visible light active two-dimensional $Cu_{2-x}S/CdS$ heterostructured nanoplate via a cation exchange reaction using roxbyite $Cu_{2-x}S/S$ nanoplate as a template. Its photocatalytic activity exhibited higher in hydrogen generation than similar compositions such as one-dimensional $Cu_{2-x}S/CdS$ nanorod system under visible light irradiation ($\lambda > 420$ nm). This work demonstrates that the two-dimensional heterostructured semiconductor nanomaterials can be the potential for efficient photocatalyst.

Poster Presentation : **INOR.P-162**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Concomitant removal of Heavy metals and Oxyanions using Iron Phosphate

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Concomitant contamination by heavy metals such as Cd, Cu, Zn, Pb and oxyanions such as As and Sb are occurred in the abandoned mine area. Soil contamination of the surrounding farmland adversely affects crops or pollutes water system. Therefore, simultaneous immobilization of metals and oxyanions are required. Since oxyanions adsorb to iron oxides and heavy metals are immobilized by phosphate, iron phosphate was selected to remove both metals and oxyanions in this study. Iron phosphate was prepared by mixing iron(III) chloride hexahydrate and sodium phosphate dibasic anhydrous. Adsorption experiments were conducted using solutions containing 5-100 mg/L of Cd, Cu and Zn and 0.5-10 mg/L As and Sb both in single and mixed metal solutions. Complex contaminated soil was treated with 1 g/kg of iron phosphate and incubated for 3 months, and bioavailable metals were analyzed every month. After adsorption remaining metal(loid) concentrations were analyzed using ICP-OES. Removal of Cd, Cu, and Zn were 12-55%, 11-58% and 5-23% with iron phosphate, respectively, which was well described by the Langmuir and Freundlich isotherm. The adsorption of Sb and As increased in the mixed metal solution compared to the single solution. Bioavailable Pb and Cd concentrations in iron phosphate amended soil decreased, but As increased, which might be attributed to substitution of adsorbed As by phosphate. Conclusively, additional studies considering the reactivity of iron and phosphate are needed, and iron phosphate can be used as a potential soil amendment for remediation of soil contaminated with heavy metals and oxyanions.

Poster Presentation : **INOR.P-163**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and characterization of volatile metal precursors for atomic layer deposition

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Thin films have many applications such as displays, photovoltaic cells, and memory devices. Thin films are manufactured by various methods such as sputtering, sol-gel method, polarization, chemical vapor deposition (CVD), and atomic layer deposition (ALD). Generally, ALD is most advanced technique for fabrication of thin films because it allows a precise control of the thickness, uniform, and conformal thin films growth. In order to form an excellent ALD thin films, suitable precursors with good volatility and stability is required. Especially, copper, zinc, germanium oxides have properties such as low cost, environmentally friendly, and reconfigurable electronic structures. Because of these properties, the oxides apply to transparent electronics, photovoltaics, sensors, memristors, electrochromics, and display backplane.Herein, we synthesized novel Cu(II), Zn(II) and Ge(II) complexes as potential precursors for ALD to form thin films. The complexes were fully characterized by 1H NMR, 13C NMR, Fourier-transform infrared spectroscopy (FT-IR), elemental analyses (EA), and thermogravimetric analysis (TGA).

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-164**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Experimental and Theoretical Studies for the Zintl Thermoelectric $Ca_{3-x}Sr_xAlSb_3$ System

Dong Hwan Seo

Chungbuk Natioanl University, Korea

Thermoelectric (TE) materials and the devices based on these materials have great potential in reducing energy crises and losses by recovering the wasted heat from various heat sources and converting it into electricity. A value indicating the efficiency of a thermoelectric material $zT = \alpha^2\sigma T / (\kappa_e + \kappa_l)$, α is the Seebeck coefficient, σ is the electrical conductivity, T is the operating temperature, κ_e is the thermal conductivity contribution from electrons and holes transporting heat, and κ_l is the thermal conductivity contribution from phonons traveling through the lattice. Zintl, good thermoelectric material in the spotlight, has complex bonding, which includes covalently bonded anionic sub-structures in a lattice of electropositive cations making high zT. Several examples of these Zintl thermoelectric materials are as follows: $A_{14}MSb_{11}$ (A = Ca, Yb; M = Mn, Al), $A_5Al_2Sb_6$ (A= Ca, Yb), $A_{11}Pn_{10}$ (A = Ca, Yb; Pn = Sb, Bi, Sn), A_2CdSb_2 (A = Ca, Yb, Eu), and A_3MSb_3(A = Ca, Sr; M = Al, Ga) series. Among the Zintl phase thermoelectric compounds, the A_3MPn_3 (A = Ca, Sr, Ba, Eu ; M = Al, Ga, In; Pn = Sb, As, P) system has been reported to have five different structure types, such as orthorhombic Ca_3AlAs_3(*Pnma*), Ba_3AlSb_3(*Cmce*), Ba_3GaSb_3(*Pnma*) and monoclinic Sr_3GaSb_3($P2_1/c$), Rb_3TiO_3($P2_1/c$). In particular, Ca_3AlSb_3 was known to have the Ca_3AlAs_3 structure type and composed of infinite chains of corner-sharing $AlSb_3$ tetrahedra. Zintl $Ca_{3-x}Sr_xAlSb_{2.7}$ synthesis was carried out by substituting Sr for Ca, and the change from Ca type to Sr type was observed and the physical properties were measured. These compounds were synthesized by the arc-melting method and their crystal structures were characterized by both powder and single-crystal X-ray diffractions. $Ca_{3-x}Sr_xAlSb_3$ system is Ca-rich compound. Quite interestingly, $Ca_{3-x}Sr_xAlSb_3$ initially crystallized in the mixed-phase, but after post-heat treatment, those were converted to the orthorhombic *Pnma* space group (Z = 4, Pearson Code *oP*28) and successfully transformed to the Ca_3AlSb_3 crystal structure. In the single-crystal X-ray diffractions data, it was confirmed that the crystal volume increased as the larger Sr was added. To understand the electronic structure of the title compounds, a series of theoretical calculations using the TB-LMTO method was performed, and the resultant DOS and

band structure analyses were thoroughly conducted. After that, the physical properties of the sample were measured using Seebeck & Electric Resistivity Measurements.

Poster Presentation : **INOR.P-165**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synergetic effects of cation substitution and *p*-type doping for thermoelectric (TE) materials: $Ca_{9-x}Yb_xZn_{4.5-y}Cu_ySb_9$ system

Naeun Seo

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Thermoelectric material is a material capable of generating electricity by using a temperature difference. The development of thermoelectric materials with high properties can use wasted heat as electricity, thereby solving the problem of global warming. The thermoelectric material can be made using the Zintl phase, which is easy to dope because it has a semiconductor property and has a complex crystal structure. Recently, One of the zintl phases, the $A_9M_4Pn_9$ (A = Ca, Yb, Eu, Sr; M = Zn, Mn) system, has been studied for the purpose of improving the TE properties by regulating the ratio of Zn. To make a new attempt, the experiment was carried out with the aim of increasing the electrical conductivity using a relatively high electronegativity of Yb by mixing Ca^{2+} with Yb^{2+}. Therefore, it was confirmed what changes in TE properties occurred due to the difference in electronegativity. In addition, by performing *p*-doping to mix Cu^{2+} with Zn^{+}, the hole concentration was also increased to obtain the overall synergistic effect as well as the effect of Ca/Yb mixing. A series of $Ca_{9-x}Yb_xZn_{4.5-y}Cu_ySb_9$ compounds were synthesized using Nb-tube, and crystal structures were analyzed through powder X-ray diffractions and single-crystal X-ray diffractions. Also, the theoretical calculation was conducted through the tight-binding linear muffin-tin orbital method, and the three structures of the DOS, COHP, and band structure were analyzed to explain the electronic structure.

Poster Presentation : **INOR.P-166**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Effect of Transition Metal Substitution for the Electronic Structure and Thermoelectric Properties of the $BaZn_{2-x}Mn_xSb_2$ System

Daewon Shim

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Thermoelectric materials can be a solution to the energy problem in modern society. Among the various thermoelectric materials, the Zintl phase can be considered as one of the best candidates. Recently, the AM_2Pn_2 (A = Mg, Ca, Sr, Ba; M = Mn, Zn, Cd; Pn = P, As, Sb, Bi) series has been extensively investigated as Zintl phase thermoelectric material, and three major structure types have been identified: the $ThCr_2Si_2$-type having metallic behavior, the $CaAl_2Si_2$-type and the $BaCu_2S_2$-type both showing the semiconducting behaviors. Interestingly, the compounds in the BaM_2Sb_2 (M = Mn, Zn, Cd) system adopted several different structure types depending on the used transition metals. For instance, $BaMn_2Sb_2$, $BaZn_2Sb_2$, and $BaCd_2Sb_2$ adopt the $ThCr_2Si_2$-type, the $BaCu_2S_2$-type, and the $CaAl_2Si_2$-type, respectively. To investigate the effect of the transition metal on the refined structure types having semiconducting behavior, the quaternary solid-solution Zintl phase $BaZn_{2-x}Mn_xSb_2$ system containing the Zn/Mn mixed-site was synthesized by the molten metal-flux method using elemental Pb, and the reactions produced large bar-shaped single crystals. The crystal structure of these products were characterized by the powder and single-crystal X-ray diffraction analysis. From the X-ray diffraction results, the structural volumes surely increase as the amount of Mn increases. A series of theoretical calculations using the $BaZn_{1.5}Mn_{0.5}Sb_2$ models were performed by the tight-binding linear muffin-tin orbital (TB-LMTO) method, and the resultant DOS and COHP curve analyses were thoroughly studied. The thermal stability of $BaZn_{1.8}Mn_{0.2}Sb_2$ was investigated by TGA, and electrical conductivity, Seebeck coefficient, power factor, and thermal diffusivity were also measured. Eventually, the experimentally obtained zT values were evaluated.

Poster Presentation : **INOR.P-167**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Effect of Sr and Cd Substitutions for the Thermoelectric and Electronic Properties of the $Ba_{1-x}Sr_xZn_{2-y}Cd_ySb_2$ System

Jiwon Jeong

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Thermoelectric (TE) materials and the devices based on these materials have been considered as one of the smartest approaches to reduce global energy consumption by recovering the waste heat from various heat sources and converting it into electricity. Zintl phase can be considered as one type of intermetallic compound composed of electropositive alkali and alkaline-earth metals elements and electronegative main-group metals or semimetal. Recently, the AM_2Pn_2 (A = Mg, Ca, Sr, Ba; M = Mn, Zn, Cd; Pn = P, As, Sb, Bi) series has been extensively investigated as Zintl phase TE materials, and three major structure types have been identified: the $ThCr_2Si_2$-type having metallic behavior, the $CaAl_2Si_2$-type and the $BaCu_2S_2$-type both showing the semiconducting behavior. To investigate the effect of cations and transition metals for the thermoelectric properties, the novel solid-solution Zintl phase $Ba_{1-x}Sr_xZn_{2-y}Cd_ySb_2$ ($0.04(1) \leq x \leq 0.09(1)$; $1.68(3) \leq y \leq 1.86(3)$) system has been synthesized by the molten Pb-flux method, and nicely grown bar-shaped single-crystals with metallic lustrous and good crystallinity were obtained from synthesis. The crystal structures were characterized by both powder and single-crystal X-ray diffractions (PXRD and SXRD). From the SXRD refinement result, we confirm that the compounds crystallized in the $BaCu_2S_2$-type structure, and the unit cell volume increases as the Cd content increases. As Ba and Sr are used as cations, the compounds adopt the Ba-type and Ca-type structures, respectively. Likewise, depending on the used transition metals, the compounds also adopt different structure types. Taking our title compounds as an example, $BaZn_2Sb_2$ and $BaCd_2Sb_2$ adopt the $BaCu_2S_2$-type and the $CaAl_2Si_2$-type, respectively. Since the $BaCu_2S_2$-type compounds have a limited tunability, we can obtain the single-phase only as the Sr and Cd are introduced below 10 % and 15 %, respectively. A series of theoretical calculations using four hypothetical models of $Ba_{1-x}Sr_xZn_{2-y}Cd_ySb_2$ was performed by the TB-LMTO method. The DOS level for $Ba_{0.5}Sr_{0.5}Zn_{1.5}Cd_{0.5}Sb_2$ was relatively lower than that of $BaZn_2Sb_2$ at the Fermi level. Electrical conductivity, Seebeck coefficient, and thermal conductivity were also measured to evaluate their thermoelectric properties. Phonon scattering was induced by the introduction of Sr and Cd, which had large atomic size differences from Ba and Zn, and this resulted in lowering thermal conductivity than that of $BaZn_2Sb_2$. Therefore, the ZT value of the title compound increases comparing to that of $BaZn_2Sb_2$ due to the effect of the lowered thermal conductivity.

Poster Presentation : **INOR.P-168**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Control of carrier characteristics through electronegativity difference in the Zintl phase thermoelectronic materials: The $Ca_{5\text{-}x\text{-}y}Yb_xEu_yAl_2Sb_6$ ($0 \leq x \leq 1.12$; $0 \leq y \leq 0.63(2)$) System

Yeongjin Hong, **Yeongjin Hong**[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Chungbuk Natioanl University, Korea*

Thermoelectric (TE) materials and devices have great potential in reducing energy crises and losses by converting wasted heat into useful energy. The $A_5M_2Pn_6$ (A = Ca, Sr, Eu, Yb; M = Al, Ga, In) series has been extensively investigated as Zintl phase TE materials. To investigate the effect by doing atoms with different electronegativites for TE properties of the $Ca_5Ga_2Sb_6$-type compounds, The title compounds were successfully synthesized by arc-melting and Pb-metal flux method. Also, their crystal structures were characterized by both powder and single-crystal X-ray diffractions. The novel Zintl phase belonging to the $Ca_{5\text{-}x\text{-}y}Yb_xEu_yAl_2Sb_6$ system was a Ca-rich compound, adopts the $Ca_5Ga_2As_6$-type structure, the orthorhombic *Pbam* space group (Z = 2, Pearson Code *oP*26). To understand the electronic structure of the title compounds, a series of theoretical calculations using the TB-LMTO method was performed, and the resultant DOS and COHP analyses were thoroughly conducted. Physical properties were measured to confirm the effect of doping Eu to Ca. As a result, compared to the undoped sample, the Eu-doped samples showed higher electrical conductivity and the Seebeck coefficient. It seems that the value of the increase in carrier mobility is larger than the decrease in carrier concentration that appears when a relatively electropositive Eu atom is substituted so that it results in higher electrical conductivity. In conclusion, higher electronic transport properties were confirmed in $Ca_{4.82(3)}Eu_{0.18}Al_2Sb_6$ and $Ca_{4.89(1)}Eu_{0.11}Al_2Sb_6$ compared with the undoped $Ca_5Al_2S_6$ samples. Also, Magnetic property measurement for $Ca_{4.37(2)}Eu_{0.63}Al_2Sb_6$, confirmed the antiferromagnetic (AFM) interactions of Eu elements at relatively low-temperature paramagnetic Curie temperatures of -29.08 K.

Poster Presentation : **INOR.P-169**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Photosensitization Process of Oligomeric Porphyrin Derivatives in Photochemical CO_2 Reduction Catalyzed by Molecular Re(I) Complex

Sunghan Choi, Daehan Lee, Min Su Choe, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Herein we report that porphyrin oligomers (**D-ZnP** and **T-ZnP**) derived from **M-ZnP** can be applied as photosensitizers in photocatalytic systems. Butadiyne-linked porphyrin oligomer has light-harvesting ability even from low-energy light source due to their extended conjugation length. Additionally, the extinction coefficient of the *Q*-band of porphyrin oligomers was increased and the absorption region of the *Q*-band was extended to the near-IR. These results support the significant improvement of the CO_2 conversion efficiency in the photocatalytic system using the porphyrin oligomer as a photosensitizer. Indeed, the photocatalytic CO_2 conversion efficiency in binary hybrid system using Re(I) doped TiO_2 is improved when using porphyrin oligomer instead of **M-ZnP**. Although the CO_2 conversion efficiency of porphyrin oligomer is relatively lowered than **M-ZnP** in the homogeneous system (Dye + Cat.) due to the lowered electron reduction power and the weaker driving force of ED ($\Delta G^* = E^{ox}$ (ED) – E^{red*}(**X-ZnPs**)), the radical anion of the porphyrin oligomer, which is generated by receiving electrons from the ED, has much higher intensity and longer lifetime than that of **M-ZnP**. This supports the rational proposal that porphyrin oligomers are good candidates as photosensitizers for dye-sensitized photocatalytic systems.

Poster Presentation : **INOR.P-170**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Photochemical CO_2-to-CO/Formate Conversion Catalyzed by Homogeneous and TiO_2-Heterogenized Cationic Half-Metallocene Ru(II)(η^6-*p*-cymene) Complex

Daehan Lee, Min Su Choe, Sunghan Choi, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

This study details the photocatalytic CO_2-to-CO or formate conversion activities of two different photocatalytic systems (IrPE + **(*p*-Cym)RuPE** and IrP/TiO2/**(*p*-Cym)RuP**) to evaluate the catalytic behavior of homogeneous and heterogenized (p-Cym)Ru(II) catalyst, respectively. A single run photolysis of the mixed homogeneous system (IrPE + **(*p*-Cym)RuPE**) in the presence of 16.7 vol % TEOA exhibited a maximal turnover number (TON) of ~800 for 48 h with a high product selectivity of formate (>79%), while the ternary hybrid system with TiO_2-immobilized **(*p*-Cym)RuP** showed the relatively higher and steady CO_2-to-CO and CO_2-to-formate conversion activities (a TON of >1660 for 100 h), reflecting the CO_2 reduction route bisected by heterogenization of **(*p*-Cym)RuP**. The mechanistic investigations along with photophysical and electrochemical studies suggests that the occurrence of MLCT ((*p*-Cym)Ru^{I}(bpy))$]^{+}$ → [(*p*-Cym)Ru^{II}($bpy^{\bullet -}$)$]^{+}$) onto the electron-withdrawing n-type TiO_2 opens catalytic route toward (*p*-Cym)Ru^{II}-COOH intermediate that results in CO_2-to-CO conversion, apart from the typical catalytic route via (*p*-Cym)Ru^{II}–H intermediate for formate production.

Poster Presentation : **INOR.P-171**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Controlled ReS_2 nanosheets attached on CdS nanorods as efficient photocatalyst for photocatalytic Hydrogen Evolution Reaction (HER)

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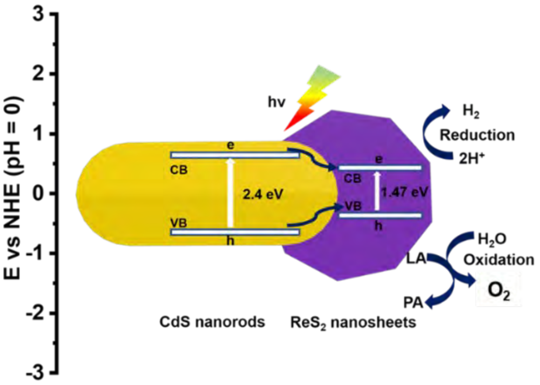
The development of highly efficient photocatalytic systems with rapid photogenerated charge separation and high surface catalytic activity is highly desirable for the storage and conversion of solar energy, Herein, a conceptionally new form of loading CdS with complementary transition-metal dichalcogenides (TMDs) semiconductors to constructs dual functional heterostructures has been widely researched as an effective strategy to improve the photocatalytic performance of CdS photocatalyst. For the TMDs cocatalyst, the MOS_2 have been widely studied and researched, however they suffer from poor catalytic activity sites/low charge transfer ability and unstable structure. In this regard's novel ReS_2 nanosheets coupled with CdS nanorods was constructed via hydrothermal route. The hybrid CdS/ReS_2-10% addressed as a promising photocatalyst for achieving excellent photocatalytic hydrogen evolution (65.650 mmol $g^{-1}h^{-1}$) without any additional redox mediator. The excellent performances are attributed due to integrates the merits of both the configuration of a heterojunction and the formation of spatially conductive network, which effectively accelerate the mobility of photoinduced carrier. The abundant catalytic activity sites on both the plane and edge of the ReS_2 cocatalyst.


E vs NHE (pH = 0)
3
2
1
0
-1
-2
-3
hv
CB
e
2.4 eV
VB
h
CB
e
1.47 eV
VB
h
H_2
Reduction
$2H^+$
H_2O
Oxidation
LA
PA
O_2
CdS nanorods
ReS_2 nanosheets

Poster Presentation : **INOR.P-172**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Investigation of structural changes and conductivity in a Ce^{3+} based metal-organic framework

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Metal-organic frameworks (MOFs), the tuneable solids constructed by metal ions and organic linkers, have captivated attention due to their high porosity and large surface areas that piloted their use in various fields such as gas storage, separation, sensor, catalysis, and drug delivery. During the last decade, MOFs have been extensively studied as solid-state electrolytes through pertinent strategies such as cation exchange, ligand and metal node functionalization, acidic and functional molecules inclusion, and defect generation.Herein, we demonstrate proton conductivity in a Ce-based MOF (CeBDC, $[Ce_6(BDC)_9(DMF)_6(H_2O)_3\cdot 3DMF]_n$) via guest inclusion. Initially, CeBDC has a 3D structure with 1D channels aligned with water and DMF molecules as a guest and coordinated solvents, indicating low porosity. However, after removing coordinated solvents at 200 °C, CeBDC can generate open-metal sites and represent the porosity with a small aperture. The activated sample shows a meta-stable structure, and the subsequent guest inclusion (H_2O, NH_4OH, and H_2O_2) indicates structural transformation due to a changed coordination environment. The CeBDC_H_2O_2 sample shows at least 2 orders of magnitude higher conductivity than the pristine sample at 298 K and 95 RH %. This research provides a possible application of CeBDC as a dopant in proton-conducting membranes, where the organic polymers often suffer from free radical damage during the operation of fuel cells.

Poster Presentation : **INOR.P-173**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Investigation of Intermolecular Enantioselective Pauson-Khand Reaction with Rhodium catalyst

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[1]*Chemistry, Queen′s University, Canada*

The enantioselective Pauson-Khand reaction, which is applied to produce chiral cyclopentenone derivatives, has been extensively studied as an intramolecular method with a molecule containing both alkene moiety and alkyne moiety. However, intermolecular Pauson-Khand reaction, using alkene and alkyne separately, has been rarely reported and has no enantioselectivity. Hence, through experiment and density functional theory (DFT), we research on the intermolecular enantioselective Pauson-Khand reaction with rhodium catalyst using chiral ligands such as BINAP or chiral diene. DFT studies revealed the reason for forming a racemic mixture without a chiral ligand. Also, the barrier of oxidative cyclization using alkyne with electron-withdrawing groups is lower than that using alkyne with electron-donating groups. The studies are in progress in computational and experimental ways.

Poster Presentation : **INOR.P-174**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

alpha-Olefin Trimerization for Lubricant Base Oils

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The demand for poly(alpha-olefin)s (PAOs), which are high-performance group IV lubricant base oils, is growing. PAOs are generally produced via the cationic oligomerization of 1-decene, which is necessarily accompanied by skeleton rearrangement deteriorating the physical properties. Consequently, transition metal-based catalytic processes with selectivity and avoidance of rearrangement can be a valuable alternative to cationic oligomerization. In this study, alpha-Olefin selective trimerization is prepared by mixing Cr complex, pyrrole, and aluminum compound, enabling the preparation of alpha-olefin trimers at ~200 g scale. As in previous study, the 1-decene trimer ($C_{30}H_{62}$) prepared after hydrogenation will show better lubricant properties than those of commercial-grade PAO-4 (kinematic viscosity at 40 °C, 100 °C, viscosity index, pour point). Moreover, 1-Octene/1-dodecene mixed co-trimers (i.e., a mixture of $C_{24}H_{50}$, $C_{28}H_{58}$, $C_{32}H_{66}$, and $C_{36}H_{74}$), generated by the selective Cr catalyst, wil exhibit outstanding lubricant properties analogous to those observed for the 1-decene trimer ($C_{30}H_{62}$).

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Poster Presentation : **INOR.P-175**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Composition of Multiple Ammonium Salts and a Salen Cobalt Complex Containing Sulfonate Anions: CO_2/Propylene Oxide Copolymerization with a Bifunctional Catalytic System

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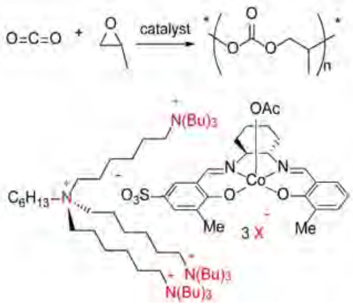
Department of molecular science and technology, Ajou University, Korea
[1]*Department of Molecular Science and Technology, Ajou University, Korea*

A (Salen)Co(III) complex, which links four quaternary ammonium salts by covalent bonds, is one of the most highly active catalysts for CO_2/epoxide copolymerization. In this work, we aimed to prepare similar (Salen)Co(III) complexes to which quaternary ammonium salts are linked via ionic interactions. Thus, we prepared multiple ammonium salts containing 2–5 quaternary ammonium salt units and (Salen)Co(III) complexes containing one or two $-SO_3^-[PhNH_3]^+$ moieties. A binary catalytic system composed of the prepared multiple ammonium salts and the prepared (Salen)Co(III) complex containing $-SO_3^-[(nBu)_4N]^+$ moieties showed high activity (TOF, 1500-4500 h^{-1}) for CO_2/propylene oxide (PO) copolymerization, whereas a combination of the multiple ammonium salts and the conventional (Salen)Co(III) complex not containing $-SO_3^-[(nBu)_4N]^+$ moieties was inactive under the identical polymerization conditions of [PO]/[Co] = 20000. However, significant amounts of cyclic carbonates were produced simultaneously, especially when using (Salen)Co(III) complexes containing two $-SO_3^-[(nBu)_4N]^+$ moieties (25–30%). This side-reaction could be mitigated by ca. 50% by using a (Salen)Co(III) complex containing one $-SO_3^-[(nBu)_4N]^+$ moiety. Cyclic carbonate formation can reasonably be attributed to the unlinked ammonium salts ($[(nBu)_4N]^+[\text{carbonate}]^-$) with the (Salen)Co(III) complex formed in the binary catalytic system.

Multiple ammonium salts containing 2-5 quaternary ammonium salt units and (Salen)Co(III) complexes containing one or two -SO_3^-[$PhNH_3$]$^+$ moieties were prepared, a combination of which showed high activity for CO_2/propylene oxide (PO) copolymerization (TOF, 1500-4500 h^{-1}).



Poster Presentation : **INOR.P-176**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Ansa-Metallocene Complexes synthesis with Thiophene-Fused Cyclopentadienyl for High-Performance Supported Catalysts.

JuYong Park, Bun Yeoul Lee[1,*]

Department of Molecular science and Technology, Ajou University, Korea
[1]*Department of Molecular Science and Technology, Ajou University, Korea*

Abstract: A series of Me_2Si-bridged ansa-zirconocene complexes coordinated by thiophene-fused cyclopentadienyl and fluorenyl ligands were prepared with an aim to develop supported catalysts adoptable in commercial process. Fluorenyl anion is more basic than thiophene-fused cyclopentadienyl, and sequence of addition to Me_2SiCl_2 was critical to achieve high yield; successive addition of fluorenyl-Li and thiophene-fused cyclopentadienyl-Li to Me_2SiCl_2 resulted in high yield (87%) whereas addition in the reverse sequence afforded the ligand precursor in low yield (27%). X-ray crystallography studies of 9 revealed that fluorenyl ligand adopts an eta 3-binding mode. Related Me_2Si-bridged ansa-zirconocene complex 15 was also synthesized replacing fluorenyl ligand in 9 with 2-methyl-4-(4-tert-butylphenyl)indenyl ligand, although obtained as a mixture of diastereomers. Furthermore, ansa-metallocene complexes 20 and 23 containing $tBuO(CH_2)_6$-tether as well as a dinuclear congener 26 were prepared by replacing Me_2Si-bridge in 12 and 15 with $tBuO(CH_2)_6(Me)Si$-bridge and connecting two complexes with $–(Me)Si(CH_2)_6Si(Me)–$ spacer, respectively. Silica supported catalysts prepared with 12, 20, and 26 containing bulky 2,7-di(tert-butyl)fluorenyl ligand showed two times higher productivity than the one prepared with the conventional $(THI)ZrCl_2$ (21-25 vs. 12 kg-PE/g-(supported catalyst)), polymers with comparable molecular weight (Mw, 330-370 vs. 300 kDa) but containing higher 1-hexene content (1.3 vs. 1.0 mol%) being produced, though the bulk density of generated polymer particles was rather inferior (0.35 vs. 0.42 g/mL).

Poster Presentation : **INOR.P-177**

Inorganic Chemistry

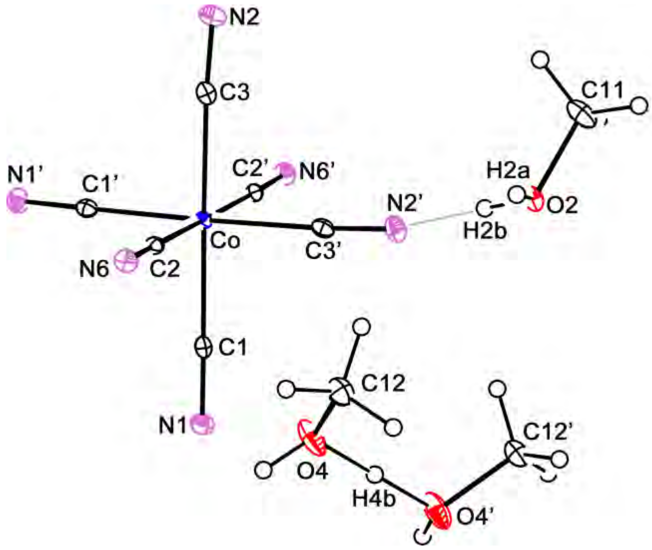
Event Hall FRI 11:00~13:00

Double Metal Cyanide Catalysts for Epoxide/CO_2 Copolymerization by using $H_3Co(CN)_6$

Yeonghyun Seo, Bun Yeoul Lee*

Department of Molecular Science and Technology, Ajou University, Korea

Double-metal cyanide complexe (DMC) is heterogeneous coordinative catalyst with activity in propylene oxide (PO) homopolymerization, but also PO/CO_2 copolymerization. The catalytic performance of DMC is sensitive to the preparation method and conditions. The preparation of conventional DMC catalysts requires mixing of $K_3Co(CN)_6$ with $ZnCl_2$ and tedious washing processes. In this work, we propose a 100 g scale synthesis of $H_3Co(CN)_6$, the structure is determined using X-ray crystallography. The new DMC catalysts prepared by mixing $H_3Co(CN)_6$ and $Zn(EH)_2$ (EH = 2-ethylhexanoate) exhibited good activity in PO homopolymerization even in the presence of a propylene glycol (PG) as a starter. A conventional DMC was inactive in the presence of such a simple PG starter. The prepared DMC was also active in PO/CO_2 copolymerization. However, we obtain low-molecular-weight macrodiol deteriorated the activity and a substantial amount of cyclic carbonate was generated (~30 wt%) in the presence of starter such as polypropylene glycol (PPG).


N2
C3
C11
N1'
C1'
C2'
N6'
H2a
N2'
O2
Co
C3'
H2b
N6
C2
C1
C12
N1
C12'
O4
H4b
O4'

Poster Presentation : **INOR.P-178**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Study on Volatile and Thermostability of Lanthanum(III) Complexes Containing Tridentate Ligands for ALD Precursors

Yongmin Go, Bo Keun Park[1,*], Taek-Mo Chung[2]

Department of Chemistry, Korea Research Institute of Chemical Technology, Korea

[1]*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

[2]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Lanthanum Oxide (La_2O_3) film has high dielectric constant (~27) and wide bandgap (~5.8eV) that could be used in MOSFETs and DRAMs. Among the many methods of depositing metal oxides, Atomic Layer Deposition (ALD) is a technology for manufacturing high-quality thin films with atomic-level precision, so it is important to develop new lanthanum precursors with volatility and thermostability for use in ALD. Therefore, we developed novel β-amino ketone tridentate ligands (ONN[Ligand1], ONO[Ligand2]) that introduced it to lanthanum complexes. Their synthesis were confirmed by ^{1}H-NMR, ^{13}CNMR, FT-IR, Element analysis (EA). Lanthanum complexes ($La(ONN)_3$,$La(ONO)_3$) were invsetigated for their thermal properties and volatile via thermogravimetric analysis (TGA) and sublimation temperature. Each substance has a similar structure, but the difference of two complexes is that the state of the substance is an oil ($La(ONN)_3$) and a solid ($La(ONO)_3$). Therefore, it is considered that both substances can be applied in various ways as ALD precursors.

Poster Presentation : **INOR.P-179**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Multi Component Organometallic Compounds, and Their Fabrication for Transition Metal Dichalcogenide Thin Film

Rosa Shin, Chang-Gyoun Kim*, Sunyoung Shin[1], Taek-Mo Chung[2]

Chemical Materials Division, Korea Research Institute of Chemical Technology, Korea
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[2]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Since 2-dimensional transition metal dichacogenide (TMDC) has various electronic structures and band gap energies according to the types of transition metals and chalcogen atoms, it is possible to implement a broadband (UV-Vis-IR) optical sensor that can selectively detect light of various wavelengths. Single source precursor for TMDC has been designed to have a ready made bonding between transition metal and chalcogen. Therefore, it has advantages such as no use of toxic H_2S gas, easy handling, and optimization of coating condition. In this study, novel single source precursors for solution processing have been designed and synthesized for the realization of high-density and high-quality van der Waals layered materials. The precursor has a chemical formular as $(Cat)_2[M^{'}Ch_4MM^{''}Ch_4]$ where Cat = Ph_4P, $M^{'}$=Mo, W,, M=Ni, Co, Pd..., $M^{''}$=Mo, W,, and Ch= S, Se. The precursors were characterized by EA, EDS, and X-ray single crystallography. The thin films were deposited by spin coating , followed by anealing based on the TGA data. The thin film was characterized by OM, XPS and et. setra.

Poster Presentation : **INOR.P-180**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and characterization of Sn precursors for atomic layer deposition

Sangmi Gu, Ji Yeon Ryu, Taek-Mo Chung[1], Bo Keun Park*

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea
[1]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

The sputtering method has fundamental problems such as difficulty in controlling the composition according to changes in the composition of the target, uniformity problems, and mass production problems. As an alternative to this, the chemical vapor deposition (CVD) and atomic layer deposition (ALD) method, which has features such as ease of composition control and uniform thin film growth, is attracting attention. However, research on n-type and p-type semiconductor materials by ALD/CVD method remains in its infancy due to the lack of development of the precursor material, an organometallic material with controlled oxidation value.Tin monoxide (SnO) and tin dioxide (SnO2) are p-type and n-type material with a wide band gap. These have excellent optical, electrical and chemical properties. It also exhibits semiconductor properties due to its low oxygen vacancies, and is attracting attention as a sensing material for gas sensors and transparent conducting oxide applications in photovoltaics and flat panel displays.Here, we synthesized a novel Sn(II) complexes as potential precursors for ALD to synthesize remarkable thin films. The complexes were characterized by Nuclear Magnetic Resonance (NMR), Elemental analyses (EA), and X-ray crystallography(XRC).

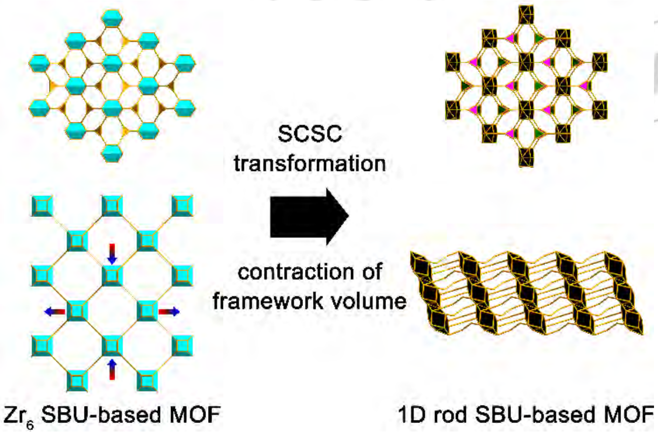
Poster Presentation : **INOR.P-181**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Transformation of a Zr_6 Metal–Organic Framework to a Rod Metal–Organic Framework

Somi Won, Junmo Seong, Dongwook Kim[1], Dohyun Moon[2], Myoung Soo Lah*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*
[2]*Beam Operation Team, Pohang Accelerator Laboratory, Korea*

A highly stable and rigid rod metal–organic framework (MOF) is obtained by the single-crystal-to-single-crystal transformation of a Zr_6 cluster-based MOF with highly interconnected but geometrically mismatched building blocks. The transformation results in a significant framework contraction, which comes from the formation of infinite chains of carboxylate- and aquo-linked Zr_6 clusters as a one-dimensional rod secondary building unit. The permanently microporous rod MOF is stable in a variety of solvents, including H_2O, and even under very harsh conditions, such as strongly acidic and basic aqueous solutions at 100 °C.



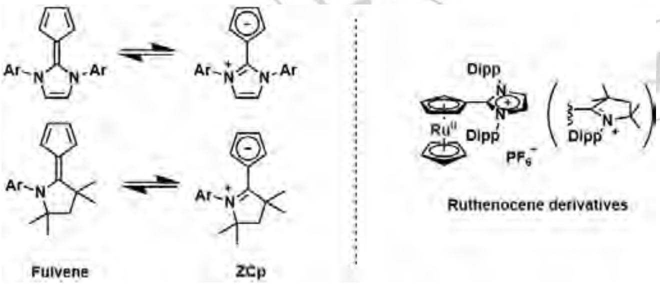
Poster Presentation : **INOR.P-182**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Air-and Moisture-Stable Zwitterionic Cyclopentadinenide Ligands and Their Ruthenocene Derivatives

Hyeonjeong Choi, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Cyclopentadienyl (CP) anion has become one of the most important ligands in organometallic chemistry. It is well known to be highly reactive due to its strong electro-donating ability. However, it is also extremely sensitive to water and air for the same reason. To control the reactivity of Cp, we synthesized new zwitterionic Cp derivatives (ZCp) by introducing pyrrolinium and imidazolium moieties. These ZCP ligands showed both air-and moisture-stability and straightforward metallation property. Also, the controlled reactivity of ZCp could make their ruthenocene derivatives achieve stable and reversible Ru(II)/Ru(I) redox states which are previously unknown. Based on the result, we have been investigating the wide range of uses of ZCP ligands. Moreover, a study about various metal complexes with ZCp ligand also will be conducted.



Poster Presentation : **INOR.P-183**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Electrocatalytic Mechanism of Hydrogen Evolution Reaction with Bioinspired Tungsten Sulfido Bis(dithiolene) Complex

Daeyong Um, Jaeheon Lee, Junhyeok Seo*

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Dihydrogen as a sustainable energy carrier attracts research attentions for establishing its production method. Electrochemical hydrogen evolution reaction (HER) should be one of the promising method to generate the gas using electric or solar energy. Current research focuses on molecular electrocatalysts of which structure is inspired by natural electrocatalysts, metalloenzymes the formate dehydrogenases. The active site of tungsten-dependent formate dehydrogenase (W-FDH) consists of a W center coordinated by an axial sulfide ligand and bis-dithiolene ligand. The redox non-innocent dithiolene coordination is essential to utilize the high-valent W(IV-VI) ion as an electrocatalytic center. The axial chalcogenide ligand also plays a role to stabilize the high-valent W center as well as to determine the selective reaction toward an incoming substrate. In general, a low-valent metal ion from the first row transition metals is employed for synthetic electrocatalysts, whereas the high-valent W ion is well used in the tungstoenzymes. In this poster, we will discuss the electrochemical behaviors of bis(dithiolene) W-sulfide complex and its application to the electrocatalytic proton reduction.

Poster Presentation : **INOR.P-184**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Temperature driven spatial distribution design of mixed building blocks in metal−organic frameworks

Junmo Seong, Seung Kyu Min*, Myoung Soo Lah*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

In the mixed building block metal-organic frameworks (MOFs), the spatial distribution of each building block should be different depending on the specific application field, so it is important to selectively control the spatial distribution. Here, we show that the reaction temperature driven spatial distribution control of mixed building blocks in a MOF using different temperature sensitivity of the diffusion coefficient and exchange rate constants of the building blocks during post-synthetic exchange (PSE) reaction. With this strategy, Core–shell microstructural and uniform microstructural MOFs can be obtained depending on PSE temperature regardless of linker exchange reaction or metal exchange reaction.

Poster Presentation : **INOR.P-185**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Activity of Ruthenium Olefin Metathesis Catalysts Bearing Indol-2-ylidene (IdY)

Minseop Kim, Hyunho Kim, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

A new class of N-heterocyclic carbene (NHCs), indol-2-ylidene (IdY), was reported in 2021 by our group. IdY showed electrophilicity and nucleophilicity both and it could form complex with transition metal such as Copper, Rhodium. Herein, IdY ligand was introduced ruthenium-based olefin metathesis catalysts, and structure was characterized by X-ray crystallography and Nuclear magnetic resonance (NMR) spectrum. Interestingly, different from CAAC-Ru catalyst, quaternary carbon of the IdY ligand is located above the benzylidene moiety. To the best of our knowledge, this conformation was first observed form for CAAC-based ruthenium catalyst. Stability test was also conducted in C6D6 40 °C, and the most stable catalyst remained about 98% after 3 weeks. Ring-close metathesis (RCM), ring-opening metathesis polymerization, and ethenolysis were conducted with IdY-Ru catalysts. Especially, the least sterically hindered catalyst (2e) showed high activity for ethenolysis for methyl oleate (TON: 74,700), and the most sterically hindered catalyst (2f) showed high activity for ROMP reaction.

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Poster Presentation : **INOR.P-186**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Ammonia synthesis by mechanochemical method under ambient conditions

Jonghoon Kim, Jong-Beom Baek[*]

Division of Energy Engineering, Ulsan National Institute of Science and Technology, Korea

Ammonia, one of the top 10 synthetic feedstocks , is mostly synthesized by the Haber–Bosch method at 400–500 °C and above 100 bar. Haber–Bosch process cannot be conducted under mild conditions for some kinetic reasons. Here, we showed that ammonia can be synthesized at mild conditons (45 °C, 1 bar) by using a mechanochemical method with iron-based catalyst. By this method, the final ammonia concentration reached 82.5 vol%, which is higher than cutting-edge ammonia synthesis under high temperature and pressure (25 vol% with 450 °C, 200 bar). The violent impact and high defect density induced by mechanochemical method on the iron catalyst were responsible for the ambientc synthesis conditions.

Poster Presentation : **INOR.P-187**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Phenanthroimidazole-based Covalent Organic Frameworks with Enhanced Activity for the Photocatalytic Hydrogen Evolution Reaction

Congxue Liu, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

The rational design of organic semiconductors based on crystalline covalent organic frameworks (COFs) as efficient photocatalysts is highly desirable. In this study, the first example of phenanthroimidazole-based COFs is reported: PIm-COF1 with an imine linkage and PIm-COF2 with a β-ketoenamine-linkage. Both COF materials showed substantial optical properties. The average hydrogen evolution rate was 7417.5 $\mu molg^{-1}h^{-1}$ for PIm-COF2, which was 20 times higher than that of PIm-COF1 (358.5 $\mu molg^{-1}h^{-1}$). This can be attributed to the strong donor-acceptor effect of PIm-COF2 and the continuous separation and transfer of the photoexcited electron-hole pair from the phenanthro[9,10-d]imidazole moiety.

Poster Presentation : **INOR.P-188**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Perylene diimide(PDI)-based organic compounds as cathode materials for highly stable lithium-ion batteries

Honggyu Seong, Joon Ha Moon, Geongil Kim, Youngho Jin, Yoon Myung[1], Chan Woong Na[1], Jaewon Choi[*]

Department of Chemistry, Gyeongsang National University, Korea
[1]*Korea Institute of Industrial Technology, Korea*

Introducing organic compounds to electrode materials instead of expensive inorganic-based materials leads to effective cost-reduction and green engineering. In this work, derivatives of amino acid substituted perylene diimide (PDI_AAs) as the redox-active organic compounds were applied for the cathode materials of Lithium-ion Batteries (LIBs). Among the as-synthesized PDI_AAs, the L-alanine substituted PDI (PDI_A) showed more improved rate capability and cycling performances of around 86 mAh/g over 150 cycles at 50 mA/g. Furthermore, at the high current density of 500 mA/g, the PDI_A exhibits a long-term cycling performance of 51 mAh/g (first discharge capacity to 131 %) over 2,000 cycles. Also, the mechanism of the charge-discharge process of the PDI_A is studied by an analysis of electrodes of the various states of charge-discharge via Ex-situ attenuated total reflection infra-red absorption spectroscopy (ATR FT-IR). Thus, PDI_A has excellent potential as cathode materials for LIBs having superior long-term cycling performances.

Poster Presentation : **INOR.P-189**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Dynamic Weak Coordination Bond of Trichloromethane Observed in a Cu-based Metal-Organic Framework: It enhances the catalytic activity of copper

Sun Ho Park, Nak Cheon Jeong[1,*]

Department of Physics & Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Physics & Chemistry, DGIST, Korea*

Coordination bondings have been extensively studied in contemporary chemistry since their nature has broadly been employed in academia and industry. Most studies of coordination bondings have been achieved only with strongly coordinating metal complexes because of their ubiquity in nature. By contrast, weak coordination bonding has been considered a polar interaction only, while studies for differing weak chemical bonds and polar interactions are challenging. Meanwhile, metal-organic frameworks (MOFs) are a structurally well-defined crystalline subset of porous materials comprising metal ions and multitopic organic linkers. Among them, paddlewheel-type MOFs with open metal sites (OMSs) such as HKUST-1 can be an excellent platform to observe the weak coordination bonding because the nanopores in the HKUST-1 can spatially confine a molecule such as a trichloromethane (TCM) that has lone-paired electrons on its neutral chlorine atom. Although the TCM has been considered as a non-Lewis-base molecule based on its chemical inertness, we postulated that the spatial confinement of TCM could enhance the probability of possible coordination of its lone-paired electrons at the metal center. In this poster, we present the existence of weak coordination bonding, demonstrating a “coordination equilibrium” that arises between the TCM and strong Lewis-base molecules such as H2O, MeOH, EtOH, DMF, and PhOH. The coordination equilibrium was demonstrated by using an in situ 1H nuclear magnetic resonance analysis. Further, Raman results that support the possible weak coordination bonding of TCM are provided.

Poster Presentation : **INOR.P-190**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Hydrophobic Pores of Metal-Organic Frameworks and Their Selective Dye Adsorption

Jiyun Kim, ChanJu Na, Younghu Son, Gyungse Park[1,*], Minyoung Yoon[*]

Department of Chemistry, Kyungpook National University, Korea

[1]*Department of Chemistry, Kunsan National University, Korea*

Among the crystalline porous materials, Metal-Organic Frameworks (MOFs) by comprising polynuclear metal clusters and organic linkers have advantages about well-defined structure. In addition, the geometrical variety of metal clusters shown different rigidity and stability of MOF structures, and by controlling this chemical nature, the chemically and thermally stable MOF has reported for applications including selective gas or vapor adsorption, separation, and catalysis. Among many applications, the selective dye adsorption in aqueous media using MOFs comprising hydrophobic ligand is rarely reported. In this study, we reported two types of Zn-SDC MOFs, which are denoted $Zn_3(SDC)_3(bpy)$ and Zn(SDC)(bpy). They were consisting of the same metal ion (Zn^{2+}) and organic ligands, stilbene dicarboxylic acid (H_2SDC) and 4,4'-bipyridine (bpy) but has different chemical formula and structure. Although the mixture phase was collected under the reported reaction condition, we prepared a pure compound of $Zn_3(SDC)_3(bpy)$ and Zn(SDC)(bpy) by controlling the ratio of organic ligands and temperature for the completely dissolving the ligands. The N_2 gas adsorption at 77K was investigated to check the properties of two structure and both uptakes were negligible. Due to the presence of hydrophobic ligands, the hydrophobic dye adsorption was investigated to Zn-SDC MOFs. $Zn_3(SDC)_3(bpy)$ with rigid trinuclear metal node showed high stability in water (at least 4 weeks) and demonstrated unique selective adsorption toward hydrophobic dye in aqueous media (Methylene Blue > Methyl Orange). Despite of the selective adsorption to hydrophobic pores, Zn(SDC)(bpy) with mononuclear metal node showed lower water stability and collapsed in aqueous dye solution. For the detailed understanding of the properties difference of two MOFs, further photochemical studies in solid-state is now in progress. Therefore, the structure and property relation of Zn-SDC MOFs was investigated and details of this work will be presented.

Poster Presentation : **INOR.P-191**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Flower- & Urchin-like $NiCo_2O_4$/NiO Nanostructures Derived from Morphology-Controlled Layered Double Hydroxides for Lithium-ion Batteries

Chanyoung Lee, Won Cheol Yoo[1,*], Sangyeop Kim[2], Jae Seong Kim[2], Deahwan Kang[2]

Department of Applied chemistry, Hanyang University, Korea
[1]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University, Korea*

Developing high-performance electrode materials with superior capacity, sustainable rate, and retentive cyclability are important for lithium-ion batteries (LIBs) in real-time applications. Binary metal oxides exhibit a high theoretical capacity (890 mAh g^{-1} of $NiCo_2O_4$) with good electrical conductivity and mechanical stability than mono metal oxides (Co_3O_4 and NiO). Still, their significant volume expansion hinders their application; therefore, several attempts have been made to overcome this issue. In this presentation, we designed unique morphologies of $NiCo_2O_4$ that could readily mitigate volume expansion, such as flower- & urchin-like morphologies with additional porosity, metal oxide nanoparticle, and carbon coating. Morphology of Ni and Co layered double hydroxide (LDH) composites was controlled by using ammonium fluoride (NH_4F) as surfactant, which were then transformed to $NiCo_2O_4$/NiO composite materials, subsequently coated with carbon. The synergistic effect between the Ni/Co elements and well-defined architecture provides large electrochemical active sites and facilitating fast ion transport and buffering volumetric change during charge/discharge when employed as anodes for LIBs.

Poster Presentation : **INOR.P-192**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Facile synthesis of cobalt-based coordination polymer

Jumin Park, Intek Song*

Department of Applied Chemistry, Andong National University, Korea

A coordination polymer is an interesting compound that have a structure in which metal-ligand-metal is continuously connected and becomes a one-dimensional(1D), two-dimensional(2D), three-dimensional(3D) coordination polymer according to the coordination polymer number.Among the various coordination polymers, $CoBr_2(pyz)_2$, $CoCl_2$(4,4'-bipy), $CoBr_2$(4,4'-bipy) has similar structures, but has different synthesis methods, which is difficult to synthesize. Therefore, we present one synthetic method using the ethanol solvent. As result, they can be synthesized very easily and simply, and seen that is well synthesized through powder x-ray diffraction.

Poster Presentation : **INOR.P-193**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

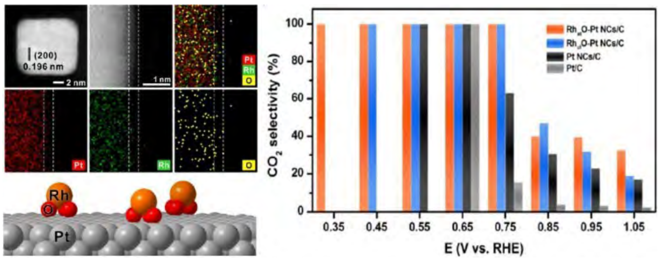
Complete Electrooxidation of Ethanol by Single Atomic Rh Decorated Pt Nanocubes

Jeonghyeon Kim, Sang-Il Choi[1,*]

Kyungpook National University, Korea

[1]*Department of Chemistry, Kyungpook National University, Korea*

The development of single site electrocatalysts, such as single atom catalyst (SAC) and single atom alloy (SAA), has demonstrated advantages of superior catalytic performance with minimized novel metal usage. However, a fundamental understanding of unalloyed single metal atom decorated on a metallic substrate is still lacking. In this work, we report unalloyed single atomic oxidized Rh on the Pt nanocube surface ($Rh_{at}O$-Pt NCs) as the electrocatalyst to achieve complete oxidation of ethanol to CO_2. X-ray absorption fine structure (XAFS) profiles and energy dispersive spectroscopy elemental mapping images demonstrate that atomic Rh was decorated on the surface of Pt nanocube with Pt-O-Rh bonding. As-prepared RhatO-Pt NCs nanocatalyst exhibits 4.2- and 11.4-fold higher current density at 0.75 V than those of Pt nanocube and commercial Pt/C. In addition, it has shown >99.9% of CO_2 selectivity in a record-low onset and wide potential region (0.35 – 0.75 V). In-situ XAFS measurements and density functional theory calculations reveal that the open Rh_{at}-O sites facilitate the C-C bond cleavage and the removal of the *CO intermediates. This work not only reveals the fundamental role of unalloyed, oxidized SAC in ethanol oxidation reaction but also offers a unique single-atom approach using low-coordination active sites on shape-controlled nanocatalysts to tune the activity and selectivity toward complicated catalytic reactions.



Poster Presentation : **INOR.P-194**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Biocompatible UV Protecting Agents based on Avobenzone Encapsulated Mesoporous Silicas

Tai yong Lee, Suk Joong Lee[*]

Department of Chemistry, Korea University, Korea

A new class of mesoporous silica (MPS) based bio-compatible UV protective materials was prepared and characterized. Avobenzone-encapsulated mesoporous silicas were modified with biphenyl-4-triethoxysilane and polyethylene glycol and their photostability under a sun-simulated lamp was tested. It was realized that the structure of material plays an important role in UV protection performance. For example, the encapsulated avobenzone enhanced the performance of absorbing UV radiations, and biphenyl layer improved the UV-blocking abilities of materials. In particular, the addition of PEG layer enriches the biocompatibility of materials. Remarkably, the SPF values were estimated to be 6.04-12.58. In vivo protection abilities were examined against sunburn developing on the skin of nude mice. The skin tissue without applying materials showed dramatically changed in the thickness of the epidermis. As a result, the skin tissue treated with UV protecting materials did not show any thickening of the epidermis, which was 14 times thinner than that of the unprotected bare skin.

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Poster Presentation : **INOR.P-195**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Functional group modification of porous organic polymers for enhanced proton conduction

Sunyoung Kim, Minjung Kang, Jong Hyeak Choe, Hongryeol Yun, Hyojin Kim, Daewon Kim, Sookyung Park, Su Min Lee, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Proton exchange membrane fuel cells (PEMFCs) have attracted considerable interest because of high conversion efficiencies and low emissions. Efficient proton conducting materials require high proton conductivity and stability under operating conditions of fuel cells. We synthesized sulfonated porous organic polymers (POPs) with modified functional groups and evaluated their proton conductivities. Through functional group modification, POPs exhibit enhanced high proton conductivity. Furthermore, POPs, which are mainly composed of C–C covalent bonds, can provide long-term stability under operating conditions. Detailed synthetic scheme and specific properties will be presented in the poster.

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Poster Presentation : **INOR.P-196**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Generation of reactive oxygen species by tetraphenylethylene-based porous organic polymers

Hongryeol Yun, Minjung Kang, Hyojin Kim, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

In many fields such as catalyst and biochemistry, an oxidant is one of the most important agents. Among them, reactive oxygen species are drawing attention because they can be produced directly from the air through a photosensitizer. Their generation is classified as type I and type II according to the pathways. We developed tetraphenylethylene-based porous organic polymers which can work as a photosensitizer and partially oxidize CEES. Their $^1O_2$ generation ability was confirmed by UV-Vis spectra with indicators, ^1H NMR, and EPR. Detailed synthetic scheme and specific properties will be presented in the poster.

Poster Presentation : **INOR.P-197**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Effect of annealing process and vacuuming process onMoS_2-based FET

Ungrae Cho, **Intek Song**[1,*]

Department of Chemistry, Andong National University, Korea

[1]*Department of Applied Chemistry, Andong National University, Korea*

Semiconductor devices based on MoS_2 have been studied a lot recently. In general, devices were made using the shadow masking method and a metal evaporator. In this method, MoS_2 can be damaged by exposure to air. So, FET was made easily and simply by using silver paste to minimize the time of exposure of MoS_2 to the air. The output curve and transfer curve before and after vacuuming process of the made FET were compared. It was confirmed that the drain current increased after vacuuming process. Also, it was confirmed that the noise was significantly reduced after annealing.

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Poster Presentation : **INOR.P-198**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Chemical and Enzymatic Conversion of Carbon Dioxide Using Biomimetic Metal Complexes

Jinheung Kim

Department of Chemistry and Nano-Science, Ewha Womans University, Korea

New mononuclear low-transition metal complexes of pyridine-2-thiolate and pyridylbenzothiazole were prepared and their reactivities studied. The two Co, Ni and Mn complexes were examined for CO2 conversion using eosin Y as a photosensitizer and triethanolamine as a sacrificial electron donor upon visible-light irradiation. Visible light-driven photoreduction of CO2 catalyzed by metal complexes affords formate with a high efficiency and a high catalytic selectivity. Undesirable proton reduction pathways were suppressed in the photocatalytic reactions with these metal catalysts under CO2. Hydrogen production under argon and kinetic isotope effects for both formate and H2 in the photocatalytic reactions are described in relation to the CO2 reduction mechanism. Further carefully designed studies expalining the selectivity of formate are necessary. Janus-type DNA nanosheets (NSs) were utilized as a support material to immobilize a Rh complex for nicotinamide adenine dinucleotide (NADH) photoregeneration and formate dehydrogenase (FDH) for CO2 reduction. The Rh complex and FDH were modified via covalent bonding using oligonucleotides, and the modified complex and FDH were successfully immobilized on the DNA NSs. This study presents the characterization results and reactivity performance of the surface-modified DNA NSs by the Rh complex and FDH immobilization.

Poster Presentation : **INOR.P-199**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

The Multi-layered SnO Nanoparticles by Annealing as High-capacity Anode Materials for Lithium Ion Batteries

So Yi Lee, Wonbin Nam, Hosung Hwang, Chan Woong Na[1], Yoon Myung[1], Jaewon Choi*

Department of Chemistry, Gyeongsang National University, Korea
[1]*Korea Institute of Industrial Technology, Korea*

The major challenge of candidate electrode materials in lithium-ion batteries (LIBs) is to solve their poor cycle stability during lithiation/delithiation and increase the electrical conductivities. Herein, The multi-layered SnO nanoparticles (SnO) with an average diameter of 200 and 220 nm used the oleylamine as surfactant at 165 ℃ and then went through an annealing process at 400 ℃ for 4 hour in Ar. The Annealed SnO has maintained its morphology. In terms of applications in LIBs, the annealed SnO has shown a remarkable improvement discharge capacity was observed as 584 mAh/g at 100 mA/g after 70 cycles. The result suggests that the annealing process is an effective way to increase the electrochemical performance of SnO anode materials in LIBs.

Poster Presentation : **INOR.P-200**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Zinc-Pyrene Porphyrin 1-D-Polymer based Photocatalyst

Gajendra Gupta, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

Among metal organic materials, coordination polymers with 1-D architectures have received considerable interests due to their aesthetic molecular structures and applications in various important fields. However, synthesizing polymers at a 1-D level with absolute precision is challenging owing to the presence of several coordination sites from the metal and the multitopic bridging ligands, which often lead to the formation of 2-D or 3-D polymers. Porphyrin and pyrene are two important widely used chromophores in metal organic synthesis with broad and significant applications. Herein, we present a one-pot synthesis of a novel linear 1-D polymer derived from porphyrin and dipyridyl pyrene ligands in the presence of zinc metal center. The 1-D polymers precipitated as single crystals. The single crystal X-ray structure exhibited an interesting morphology with zinc metal coordinated to the porphyrin center, which was further bonded to the pyrene ligand, resulting in a linear 1-D-type polymer, with repeated Pyr-ZnTPP-Pyr units (Figure 1). The photophysical properties of the polymer were studied in detail. The polymer has the ability to harvest light as confirmed by time correlated single photon counting and confocal laser scanning microscopy studies. In addition, it also showed excellent catalytic activity toward photooxidation of 1,5-dihydroxynaphthalene (DHN) to 5-hydroxy-1,4-naphthaquinone (Juglone) with a conversion rate of around 95%

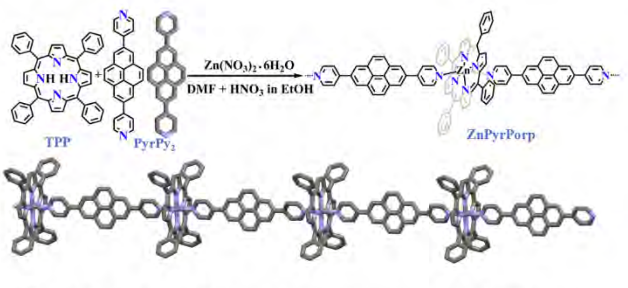

Figure 1: Scheme showing the formation of ZnPyrPorp polymer and its SCXRD structure.

Poster Presentation : **INOR.P-201**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Photocatalytic Degradation of a Sulfur Mustard Simulant using Porous Organic Polymer Composite

Hyojin Kim, Minjung Kang, Jong Hyeak Choe, Hongryeol Yun, Sunyoung Kim, Su Min Lee[1], Sookyung Park[1], Chang Seop Hong*

Department of Chemistry, Korea University, Korea

[1]*Korea University, Korea*

Porous materials have recently attracted considerable attention as efficient photosensitizers for the photocatalytic degradation of toxic chemicals. Herein, a novel type of porous organic polymer (POP) photosensitizer was developed using straightforward one-pot polymerization. Moreover, POP was subjected to material diversification using a substrate for practical applications. Photophysical properties of POP and POP-based composite were examined by UV-Vis absorbance spectra and EPR spectra. Subsequently, photodegradation of a sulfur mustard simulant using POP and POP-based composite under ambient environments is demonstrated, showing promising utility in real-world applications. Detailed synthetic scheme and characterization will be presented in the poster.

Poster Presentation : **INOR.P-202**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Photocatalytic performance via C_{60}-incorporated Nano Mixed Ligand MOFs (nMLM)

Woo Seong Jo, Chang Yeon Lee[*]

Department of Energy and Chemical Engineering, Incheon National University, Korea

Photocatalytic reaction using energy from the infinite sunlight is being used for environmentally friendly CO_2 reduction, and decomposition of organic pollutants, and hydrogen production. Light is irradiated to the photosensitizer to generate electron-hole pair, and the photosensitizer in an excited state transfers energy to triplet oxygen to generate reactive oxygen species (ROS). In order to effectively produce these ROS, electron-hole recombination must be minimized in the photocatalyst, and the catalyst must be able to absorb light in a wide range. The best way to obtain these conditions is to mimic the natural photosynthetic system. Designing and synthesizing the ordered light-harvesting systems possessing complementary absorption and energy-transfer process between chromophores, are essential steps to accomplish mimicking of the natural photosynthetic system. A new class of organic and inorganic composite metal–organic frameworks (MOFs) has emerged as an essential material for numerous applications, including photocatalytic hydrogen generation. Recently, we developed a nanosize mixed-ligand MOF (nMLM) by reacting a Zr metal source with a mixture of pyrene and porphyrin building units which showed superior photocatalytic performance. Herein, we further constructed a three-stage EnT (Energy transfer), ET (Electron Transfer) acceptor and donor by SALI (Solvent-Assisted Ligand Incorporation) of C_{60} to nMLM. This prevents electron-hole recombination and shows high efficiency. The C_{60} nMLM Triad system which mimics the natural photosynthetic process showing excellent photocatalytic performance.

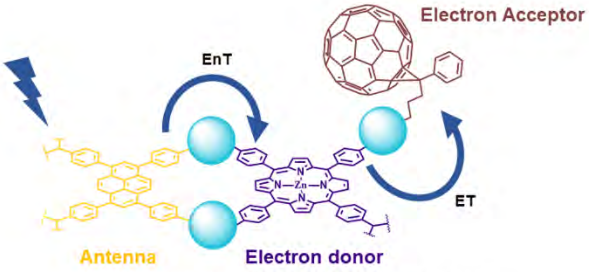

Figure 1 C_{60}nMLM triad EnT and ET system

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Poster Presentation : **INOR.P-203**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

degradable filter with pcl

Yeon Park, Kang Hyun Park[1,*]

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This work highlights the use of Poly-Caprolacton for making biodegradable filter with the method of electrospinning. The concept is appropriate to the world, where the impact of plastic pollution on environment is a persistent challenge. In this study, chloroform and N,N-dimethylformamide were prepared for using as solvent. The result of SEM prove that filter has successfully synthesized through the smooth surface and consistent thickness of nanofiber.

Poster Presentation : **INOR.P-204**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

New imidoyl based radical platform using N-heterocyclic carbene

Seoung Su Kim, Eunsung Lee[1,*]

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[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Organic radicals can be utilized as not only building blocks with their high reactivity but also materials themselves in molecular magnets, batteries or as catalysts. Despite increasing interests in organic radicals, only few types of them are isolated and used these days since most radicals decompose easily. N-heterocyclic carbenes (NHCs) have been considered as major candidate in p-block stabilizing with their strong sigma-donability and pi-acceptability. We have been develop several organic radicals stabilized by NHCs. Here we suggest new imidoyl based radical platform using NHC that can introduce diverse aromatic functional groups.

Poster Presentation : **INOR.P-205**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Solvent-assisted Reversible Interpenetration of a Cu Paddlewheel-based Metal-organic Framework

Cheol Yeong Heo, Nak Cheon Jeong*

Department of Physics & Chemistry, DGIST, Korea

Metal-organic frameworks (MOFs), extended network consisting of metal ions (or metal-oxo clusters) and multitopic organic ligands have studied since their attractive properties such as porosity, modularity, and crystallinity. These properties give them potential functions in various fields such as gas absorption, catalysis, molecular separation, drug delivery, and sensing.MOFs with large open cavities could easily form thermodynamically stable interpenetrated framework, leading to the reducing their porosities. Although it is preferred for such applications that MOFs possess non-interpenetrated framework, interpenetrated MOFs have shown specific, selective absorption performance. So far, the control of interpenetration in MOFs and structural dynamism for MOFs have been intensively studied to achieve the desired structure. Structural transformation of MOFs could be triggered by various external stimuli such as pressure, light, heat, and guest molecules. Isolation of each single frameworks must involve the breakage of chemical bond of single framework. To the best of our knowledge, reversible structural transformation under mild condition is rarely reported.In this presentation, we show the reversible post-synthetic transformation reaction between the thermodynamically less stable non-interpenetrated framework of MOF-143 and thermodynamically more stable doubly interpenetrated framework of MOF-14. The transformation of MOF-143 to MOF-14 was preformed through the exchange of protic solvents at room temperature, whereas the reverse transformation was conducted in the presence of pyridine and DMF at100 °C. We believe that our observation and demonstration can aid in understanding the assembly and disassembly nature of framework.

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Poster Presentation : **INOR.P-206**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Highly Selective and Durable Photochemical CO_2 Reduction by Polymeric P3HT-Sensitized TiO_2 Catalyst

Min Su Choe, Daehan Lee, Sunghan Choi, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son[*]

Department of Advanced Materials Chemistry, Korea University, Korea

Herein, we report a detailed investigation of efficient hybrid photocatalyst system for carbon dioxide reduction. The system is based on a co-assembly of conjugated polymer photosensitizer (**P3HT**) and molecular Re(I) reduction catalyst on TiO_2 semiconductor. The hybrid system consists of **P3HT** (poly(3-hexylthiophene-2,5-diyl)) as a visible-light photosensitizer and *fac*-[Re(4,4′-bis(methylphosphonic acid)-2,2′-bipyridine)$(CO)_3Cl$] as a CO_2 reduction catalyst (ReP). The **P3HT** photosensitizer is coated onto Re(I) catalyst (ReP)-loaded TiO_2 particles to build up a new polymer-sensitized TiO_2 photocatalyst system (**P3HT**/TiO_2/ReP). The **P3HT**-based hybrid system showed the most durable catalytic activities compared to our previous ternary systems using molecular photosensitizer. Under irradiation with low energy light (>500 nm), the hybrid **P3HT**/TiO_2/ReP catalyst showed a TON of ~5300 over an extended time period of 830 h.

Poster Presentation : **INOR.P-207**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Nickel-Catalyzed NO Group Transfer Coupled with NO_x Conversion

Sudakar Padmanaban, **Yunho Lee**[1,*]

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[1]*Department of Chemistry, Seoul National University, Korea*

The different forms of nitrogen oxides (NO_x) are serious environmental pollutants due to human activity. NO_x conversion is, therefore, an important process for balancing the global nitrogen cycle. Distinct from the biological NO_x transformation, we have devised a synthetic approach to this Issue by utilizing a bifunctional metal catalyst for producing value-added products from NO_x. Here, we present a novel catalysis based on a Ni pincer system, effectively converting Ni–NO_x to Ni–NO via deoxygenation with CO(g) in a stepwise manner and acts as an efficient catalyst for transferring the so-formed nitroso group from the Ni–NO moiety to alkyl halides which in turn forms oxime compounds. Successful catalytic production of oximes from benzyl halides using $NaNO_2$ is presented with a turnover number of >200 under mild conditions. In a key step of the catalysis, a nickel(I)–•NO species effectively activates alkyl halides, which is carefully evaluated by both experimental and theoretical methods. Our nickel catalyst effectively fulfills a dual purpose, namely deoxygenating NO_x and catalyzing C–N coupling. This novel NO_x conversion and utilization (NCU) technology is a step toward achieving a sustainable N-neutral chemical industry.

Poster Presentation : **INOR.P-208**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Reduction of Ag^+ Ion and Chemical Change of Functionalized Amine during Impregnation Process

Jeong Woo Hong, Hee-Jung Im*

Department of Chemistry, Jeju National University, Korea

Ag^+ ions underwent chemical reduction without any reducing agent in this study. This tendency can observe when Ag^+ ions are surrounded by the specific concentration of amines. To investigate the Ag^+ ion reduction, propylethylenediamine and mercaptopropyl ligand functionalized silica gels were prepared and added into Ag^+ ion solution (; $AgNO_3$ or Ag_2SO_4 solution). In addition, Ag nanoparticle solutions were prepared for comparison with the impregnation tendency of the Ag^+ ion solutions. In the case of mercaptopropyl functionalized silica gels, predictable and unremarkable results were obtained. On the contrary, Ag^+ ions formed Ag_4^{2+} clusters which were observed through UV-vis and XPS spectra during impregnation process into the propylethylenediamine ligand functionalized silica gels. In addition, functionalized amines underwent chemical changes to form amide group. This change was not detected at previous studies. Therefore, it is necessary to investigate the mechanism of this tendency.

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Poster Presentation : **INOR.P-209**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Synthesis of Sterically Less Hindered Triazenyl Radical Stabilized by N-Heterocyclic Carbenes

Jaelim Kim, Eunsung Lee[*]

Department of Chemistry, Pohang University of Science and Technology, Korea

Organic radicals have great attention up to date because of their unique electronic properties and synthetic challenge. Recently, our group first reported the triazenyl radicals stabilized by the N-heterocyclic carbenes (NHCs)1. However, these radicals showed only single-electron transfer toward various transition-metals, and electrophiles. We proposed these limited reactivities were caused by steric hindrance nearby triazenyl cores from several types of research about radicals derived from Frustrated Lewis Pairs (FLPs)2.Herein, we reported the triazenyl radical stabilized by the smallest NHCs. Despite weaker π-accepting properties and smaller steric effects, the introduction of the sterically less demanding NHC (IMe) to the organic radicals could support obtaining a stable redox-cycle, which is attributed to that π-accepting ability of NHCs delocalizes the radical's spin density onto the carbene moiety. The detailed synthesis and full characterization of the radical including X-ray determined structure and EPR spectroscopy will be presented.

Poster Presentation : **INOR.P-210**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Study on Dye-Sensitized Solar Cell Using Fruit Extracts

Chaeyoung Moon, Jeong Woo Hong[1], Hee-Jung Im[1,*]

Department of Chemistry & Cosmetics, Jeju National University, Korea
[1]*Department of Chemistry, Jeju National University, Korea*

Dye-sensitized solar cells are attracting attention due to various advantages such as price and maintenance of initial efficiency. However, commercialization is difficult because of efficiency aspects or material instability. To compensate for this, many studies are being conducted for each material of the dye-sensitized solar cell (DSSC). In this study, the efficiency of solar cells was investigated by changing the dye. The dyes used are berry, 'Pootgyul' (Immature Fruit of Satsuma Mandarin) and lemon extracts. Berry extract was used as control as its efficacy was investigated in several studies. As a result of measuring the voltages, the voltage of the berry extract was measured to be the highest. Pootgyul and lemon extracts obtained similar values. It was lower than that of berry extract, but there was no significant difference. To learn more about this, the absorbance of both extracts was measured. The peak positions of the two extracts were similar. It can be seen that the similarity of the voltage measurement results of pootgyul and lemon extracts is related to the absorbance measurement results.

Poster Presentation : **INOR.P-211**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Introduction of Guanidinium into Perovskite Nanocrystals for Efficient and Stable Light Emitting Diodes

Dohyun Jeon, Bonju Koo[1], Jaemin Lee[1], Tae Kyu Kim[*], Seon Joo Lee[1,*]

Department of Chemistry, Yonsei University, Korea
[1]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

ABX_3 perovskite nanocrystals (PNCs) with inorganic A cation ensure high stability against moisture and heat. However, it usually decreases the luminescence properties because of its relatively small radius. Here, we successfully synthesized triple-cation PNCs including both organic and inorganic A cations via room temperature-based synthetic method. Incorporation of guanidinium (GA) into $Cs_{0.85}FA_{0.15}PbBr_3$ PNCs improves photoluminescence quantum yield (PLQY) by 90.1%. Due to the strong hydrogen bonding effect, GA suppresses surface defects and enhances the photoluminescence lifetime of PNCs. By tuning the GA ratio, we can realize light-emitting diodes (LEDs) with sharp green electroluminescence at 515 nm, external quantum efficiency (EQE) of 13.06%, and luminance of 20,192 cd m^{-2}. Moreover, triple-cation PNCs-based LEDs including GA exhibit a significant increase in a lifetime by 7.47-fold than that of $CsPbBr_3$ PNCs-based LEDs.

Poster Presentation : **INOR.P-212**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Polymerization of Methyl Methacrylate by Precatalyst Palladium(II) Complexes

Hyosun Lee

Department of Chemistry, Kyungpook National University, Korea

The reaction of **$[PdCl_2\cdot(MeCN)_2]$** with N-substituted N,N'-bidentate imino-pyridine ligands ($L_n = L_A – L_C$) where L_A is (E)-3-methoxy-N-(quinolin-2-ylmethylene)propan-1-amine, L_B is (E)-N-(pyridin-2-ylmethylene)hexan-1-amine, and L_C is ((E)-3-methoxy-N-(pyridin-2-ylmethylene)propan-1-amine, gave Pd(II) complexes **$[L_nPdCl_2]$**, respectively. All complexes were characterized by ^{1}H-NMR, ^{13}C-NMR, IR, and elemental analyzer. The molecular structures of Pd(II) complexes were characterized by X-ray single crystal diffraction. The catalytic properties of these complexes toward the polymerization of methyl methacrylate in the presence of MMAO by of all complexes was investigated at 60 ^{o}C.

Poster Presentation : **INOR.P-213**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Acetylene Separation from Carbon Dioxide and Ethylene by bimetallic imidazolium-based Metal-organic Frameworks

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Department of Chemistry, Pohang University of Science and Technology, Korea

Acetylene separation from carbon dioxide and ethylene is challenging because of their similar sizes and physical properties. Metal-organic frameworks (MOFs) in general present themselves to be strong candidates for these separations owing to the presence of functional pore surfaces that can selectively capture a specific target molecule. Herein, we report the bimetallic imidazolium-based MOFs, JCM-1s, which have isostructural with previously reported MOF, JCM-1(Co). The selective sorption of acetylene over carbon dioxide and ethylene in JCM-1s was successfully demonstrated by the equilibrium gas adsorption analysis. Furthermore, its excellent hydrolytic stability enabled the separation processes highly recyclable without a substantial loss in acetylene uptake capacity.

Poster Presentation : **INOR.P-214**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Mechanically Responsive Porphyrinic Metal-Organic Frameworks

Joohan Nam, Wonyoung Choe*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Flexible metal-organic framework (MOF) has become a prominent member of stimuli-responsive materials, due to their highly deformable nature, which made them promising materials for diverse applications. Beyond the pre-developed flexible MOFs, chemists have tried to carefully control the deformable nature of MOFs toward property optimization. For sophisticated control of flexibility, a clear distinction between flexible points and rigid parts is essential, as exemplified by hinged MOFs. Hinged MOFs have a clear structural heterogeneity and dynamics, in which the molecular origin of the flexibility can be easily identified as a hinged point. However, studies on tuning the flexibility of hinged MOF backbones have been active only for some well-known MOFs, especially MIL-53. In this presentation, we show a series of CdSO4-type hinged MOFs varying the coordinated halogens to the metal node. Throughout the series, their symmetry, hinge angle, and mechanism of hinged motions are various, and the crystallographic information is obtained by temperature-dependent synchrotron single-crystal X-ray diffraction.

Poster Presentation : **INOR.P-215**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Geometry Isomer Effects for MLCT and $\text{ICT}_{\textbf{Ligand}}$ Character in the Cyclometalated Pt(II) Complexes

Minjung Chae, Kyung-Ryang Wee*

Department of Chemistry, Daegu University, Korea

Based on the previous research, the ICT characters depend on terphenyl isomer effects in the triphenylamine as a donor (D), imidazole as an acceptor (A), and terphenyl as an π-linker containing D-π-A dyads were studied and characterized to confirm the emission origin. We have designed and prepared a series of D-π-A ligand containing Pt complexes (**O**, **M**, and **P**) with a π-A ligand containing **IMI** as reference material to investigate structure-photophysical properties relationships. Especially, we tried to understand MLCT characters depending on the geometric effect of ortho-, meta-, and para-terphenyl isomer in the Pt complexes. The 4-coordinate square planar structure of **O**, **P**, and **IMI** complexes were confirmed by SC-XRD crystallography. In the absorption spectrum, the wavelength band at < 400 nm for all complex corresponds to the ^{1}LC and ^{1}MLCT with each ICT character. The absorption wavelength appears > 400 nm is ^{3}MLCT or ^{3}LC. The emission spectra of the **O**, **M**, and **IMI** complexes showed a similar emission maximum of 525 nm indicating ^{3}MLCT emission. Also, for **P**, the emission of ICT was additionally observed near 475 nm and it shows red-shifted characters as the solvent polarity increased, which is indicated ICT emission. In particular, in the solid-state, we have observed systematic red shifting emissions in the order of **O** < **M**, **IMI** < **P**. In addition, the electrochemical experiments showed different redox properties according to the structural characteristics, and these results were well matched with the DFT calculation. As a result, we suggest the Pt complex MLCT character can be controlled by ligand geometry isomers.

Poster Presentation : **INOR.P-216**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

The role of organic building unit symmetry in UiO-type metal-organic frameworks

Hyeonsoo Cho, Sunwoo Lee[1,*], Wonyoung Choe[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Chonnam National University, Korea*

Reticular chemistry is a useful roadmap to guide metal-organic frameworks (MOFs) with diverse building units and topologies. Especially, the symmetric building unit is generally used to construct MOFs due to high designability and predictability. However, diversifying symmetric building units with functionalization is already enough established. Therefore, the asymmetric organic building units unveil the potential of the directional property. In this study, we investigated the role of the asymmetric organic building unit in UiO-type MOF.

Poster Presentation : **INOR.P-217**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

A Detailed Evaluation for Ultrafast Excited State Relaxation Dynamics of Nonradiative Process for Blue Phosphorescent Cyclometalated Ir(III) Complexes Using Femtosecond X-ray Transient Absorption Spectroscopy

Mina Ahn, Kyung-Ryang Wee*

Department of Chemistry, Daegu University, Korea

Research on cyclometalated Ir(III) complexes, which can be classified as homoleptic or heteroleptic, have been a hot topic because of their efficient emission, excellent thermal stability, and wide variety of tunable emission colors and promising applications in a highly efficient electrophosphorescent organic light-emitting diode (OLED). So far, most reports have argued that cyclometalated Ir(III) complexes with low emission efficiency undergo a nonradiative process by Ir-N bond rupture of cyclometalating ligands that occurs during the photoexcitation process, but experimental evidence is lacking. To understand the intrinsic nature of nonradiative process, we investigated the excited state relaxation dynamics of a heteroleptic Ir(III) complex, *fac*-Ir(ppy)$_2$(ppz), and two homoleptic Ir(III) complexes, *fac*-Ir(ppy)$_3$ and *fac*-Ir(ppz)$_3$, using femtosecond X-ray transient absorption (fs-XTA) spectroscopy, ultrafast optical transient absorption (TA) spectroscopy, and DFT/TDDFT calculation. Both fs-XTA and TA data demonstrate that the ultrafast relaxation dynamics of ~450 fs is due to internal conversion (IC) from $^{3}\mathrm{ML_{ppz}CT}$ to $^{3}\mathrm{ML_{ppy}CT}$, rather than the nonradiative process from the ^{3}MLCT state to the ^{3}MC state. This fast IC is the first example observed in Ir(III) complexes that $^{3}\mathrm{ML_{ppz}CT}$ state generated by the spin-forbidden transition rapidly relaxes to $^{3}\mathrm{ML_{ppy}CT}$ through the IC process, which is observed only in *fac*-Ir(ppy)$_2$(ppz) but not in the homoleptic Ir(III) complexes. The DFT/TDDFT calculations support that the abnormally fast IC for *fac*-Ir(ppy)$_2$(ppz) is due to a large nonadiabatic coupling and the small energy gap between the two states.

Poster Presentation : **INOR.P-218**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Design Strategies of Zr-, V-Based Metal-Organic Polyhedra

Eunjie Ju, Jiyeon Kim, Wonyoung Choe*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Metal-organic polyhedra (MOPs) are one of the metal-organic materials (MOMs). Thanks to their solubility, MOPs have been utilized for solution-based applications, such as membrane separation and homogeneous catalysis, which cannot be achieved by extended materials, i.e., porous solids. Unlike porous solids, the modular design of cage structures can provide precisely designed intrinsic pores. Currently, various cage structures have been reported with affluent choice of building blocks, i.e., metal clusters and organic ligands. In this presentation, we study distinct cage structures and their design strategies of Zr- and V-based MOPs, especially focused on 3-connectivity of metal clusters (Figure 1a). Even though Zr-, and V-based clusters have same connectivity, the different types of cages are produced. We are looking at the phenomenon in terms of angle and steric. According to CSD reports to date, Zr-MOPs have tetrahedron (M_4L_6 or M_4L_4), cube (M_8L_{12}), square (M_4L_6), triangle (M_3L_3) and cocoon (M_2L_3) types of cages, and VMOPs have tetrahedron (M_4L_6 or M_4L_4) and cube (M_8L_6) types of cages, with the combinations of cluster (M, blue and light green) and carboxylate-based ligands (L, white) (Figure 1b). We propose the sophisticated strategy to predict cage design.

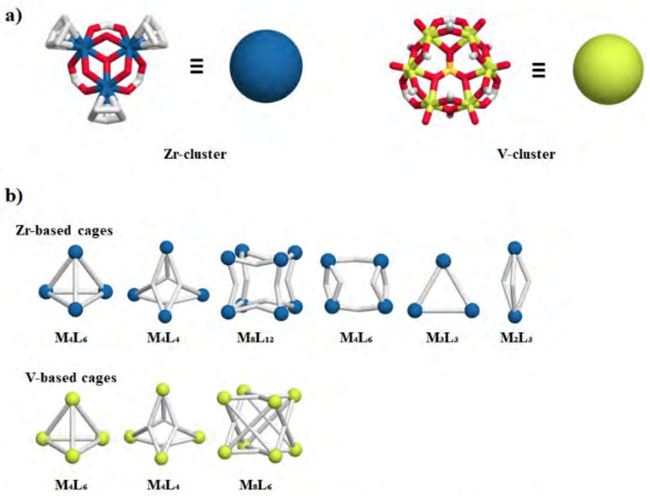

Figure 1. a) Zr- and V-based clusters and b) Zr- and V-based Cages

Poster Presentation : **INOR.P-219**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Influence of Ancillary Ligand on Photophysical Properties in the Heteroleptic Phenylpyrazole Iridium Complex

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[1]*Department of Chemistry , Daegu University, Korea*

Heteroleptic iridium(III) complexes were investigated by many researchers because of their high phosphorescence efficiency and the easy tuning of emission color by the ancillary ligands. In this study, we synthesized homoleptic ***facial*** **Ir(ppz)3** (ppz = phenylpyrazole) and a series of heteroleptic **Ir(ppz)2(N^O)** (N^O = pyridine carboxylic acid, hydroxypyridine carboxylic acid, and isoquinoline carboxylic acid) to investigate the influence of ancillary ligand for the photophysical properties. The **Ir(ppz)3** showed deep-blue emission with a vibronic structure at 77K, while **Ir(ppz)2(N^O)** showed broad and red-shifted emission spectra. Also, we have investigated electrochemical properties by cyclic voltammetry (CV) and the theoretical calculations using density functional theory to understand the effect of ancillary ligands on the emission changes. Since the triplet MLCT state of main ligand was calculated to be higher than the triplet MLCT state of ancillary ligand, ILET between the main ligand and the ancillary ligand may occur exothermically in the triplet state. The dynamics of the ILET were monitored directly using a transient absorption (TA) spectroscopic technique. As the time delay increase, intensity of TA band for the triplet MLCT state of ancillary ligand increase and decrease. It has been proven that the ILET phenomenon occurs using TA spectroscopy. Additionally, **Ir(ppz)2(N^O) (N^O = hydroxypyridine carboxylic acid)** showed long-lived TA species, attributed to excited-state intramolecular proton transfer (ESIPT).

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Poster Presentation : **INOR.P-220**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Phase Control of Zr-Based Metal-Organic Polyhedra

<u>Changhyeon Cho</u>, Eunjie Ju, Jiyeon Kim, Wonyoung Choe*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Metal-organic polyhedra (MOPs) are an emerging class of porous materials due to their processibility and intrinsic porosity. In particular, Zr-based MOPs are attracting attention for their outstanding stability, leading to practical applications such as gas adsorption, molecular separation, and desalination. Although optimizing pore size would be essential for the applications, the inclusion of large pores in Zr-MOPs remains a daunting challenge. When extended ligands are used for the synthesis of a large cage, the formation of large tetrahedral MOPs was hindered and cocoon-type MOPs with small cavities were produced (Figure 1). There was an attempt to create tetrahedron MOPs using extended ligands with bulky functional groups. However, the bulky functional groups blocked the window of the pores. In this presentation, we adopted a two-step synthetic strategy to control the competing products, tetrahedral versus cocoon-type MOPs, and unveiled the kinetic and thermodynamic products in polymorphic Zr-MOPs by controlling synthetic parameters. Two-step synthesis can be a simple yet powerful strategy for producing large tetrahedral MOPs in pure phase.

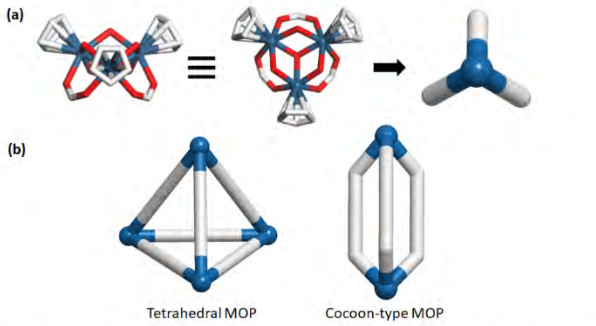

Figure 1. Structure of Zr-based metal-organic polyhedra (MOPs). (a) structure of Zr cluster. (b) Tetrahedral and cocoon-type Zr-MOPs.

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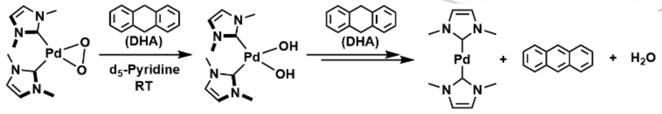
Poster Presentation : **INOR.P-221**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Oxygen Reduction via Palladium mediated C-H Activation: Formation of the Monometallic Palladium(II) Dihydroxide Complex as an Intermediate

Jeongmin Cha, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Palladium-mediated oxidative transformations using molecular oxygen (O2) have been studied in the perspective of preparing oxidized organic substrates or the development of renewable energy systems such as fuel cells. Pd-mediated O2 reduction to water via C-H activation of the 9,10-dihydroanthracene is described in present work. The reaction was monitored and found to have unusual sigmoidal kinetic profiles, with a monometallic Pd-dihydroxide complex serving as an intermediate. The dihydroxide complex was synthesized and described separately, with X-ray crystallography revealing that the two hydroxide ligands were cis-positioned. The dihydroxide complex's intermediacy was tested by mediating the C-H activation of the 9,10-dihydroanthracene. The entire reaction mechanism was suggested by DFT calculations, which revealed that the initial HAT's high activation barrier was ascribed to the induction phase, while the in situ produced dihydroxide and dimeric peroxide complexes led to the burst period.



Poster Presentation : **INOR.P-222**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Microwave synthesis of Ln-ReO_x as a highly efficient RGB phosphorescent

Jongwon Oh, Seok Min Yoon*

Department of Chemistry, Wonkwang University, Korea

We successfully synthesized novel phosphorescent crystalline materials, which are lanthanides incorporated rhenium oxide (Ln-ReO_x, Ln=Eu, Tb) by microwave-synthesis with a reaction time of only 2min. The Ln-ReO_x can be prepared as a crystalline film by spin-coating, and they emitted red, green, and blue phosphorescence interestingly. Eu-ReO_x emitted red emission, and Tb-ReO_x emitted green and blue emission. Eu-ReO_x film showed the significant photoluminescence (PL) spectrum peak at 617nm corresponding to red and Tb-ReO_x film showed the spectrum at 545nm and 488nm. The lifetime of red and green emissions are 500μm and 856μm respectively. Moreover, the photoluminescence quantum yield (PLQY) of both Eu-ReO_x and Tb-ReO_x are around 10%, although PLQY of most transition metal-oxide film phosphorescents has lower than 5 %. Furthermore, blending Eu-ReO_x and Tb-ReO_x crystalline film exhibits white light emission. In addition, Ln-ReO_x films can be deposited on flexible polymer substrates like PET, and they can stably emit their PL properties even after 1000 times mechanical bending or wrinkling.

Poster Presentation : **INOR.P-223**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Novel Tungsten Precursors Containing Amido Ligands for W-based Thin Film

JiYoung Son, Bo Keun Park[1,*], Chang Seop Hong[*], Taek-Mo Chung[2], Ji Yeon Ryu[1]

Department of Chemistry, Korea University, Korea

[1]*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

[2]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Tungsten(W) is a material that has low ohmic contact resistance and good step coverage, high electrical conductivity, superior thermal stability and high corrosion resistance. Due to these qualities, W–based thin films (ex, W, its Nitrides, Oxides, Sulfides, Carbides) have been widely used in a myriad of technological applications in areas including semiconductor metallization, gas sensing, catalysts, energy storage, solid lubricants. WF_6 has been widely used for W thin films in CVD, ALD process due to its high vapor pressure and gas phase at room temperature. However, WF_6 revealed problems that this precursor incorporates corrosive halogen impurities in the form of HF as a byproduct, resulting reacting with the underlying materials and damaging substrate. Herein, we focused on development of precursors for halogen free tungsten precursors for W-based thin films. We will present the synthesis of novel W amido compounds, as precursors for W-based thin films and their structural characterization and thermal properties by spectroscopic methods (^{1}H NMR, ^{13}C NMR, FT-IR) , X-ray single crystallography, thermogravimetric analyses (TGA). Also we carried out a deposition test in our laboratory and other research teams.

Poster Presentation : **INOR.P-224**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Palladium doped Rhenium Oxide catalyst for methanol steam reforming

Gyeong eun Hyun, Seok Min Yoon*

Department of Chemistry, Wonkwang University, Korea

Rhenium (Re) has been used as a mechanically substantial component to make jet engines due to their extremely high mechanical stability, when it forms superalloy with other metals. Also, the Re has been fascinated to utilize as a catalyst for olefin metathesis and hydrogenation. Practically, Re-Ni alloy is a widespread catalyst used in the petroleum refinery process. Nevertheless, in academia, the heterogeneous catalytic potential of the Re is still not studied well. Thus, to discover heterogeneous catalytic performance of the Re, we tried to apply synthesized novel Pd doped mixed-valence Re-oxides (Pd@MVReO$_x$) as an efficient catalyst for decomposing methanol (CH_3OH) to produce hydrogen (H_2) gas. Methanol can be a promising hydrogen fuel due to its high hydrogen content 12.5wt% and easy transportation and storage.[1] Re can be a sustainable catalyst to decompose the methanol and produce H_2 gas from it. Pd@MVReO$_x$ catalysts were synthesized by simple solvothermal methods. The Pd@MVReO$_x$ were synthesized as crystallites with cube-shaped morphology and their oxidation states were controlled by annealing temperature. The optimized Pd@ReO$_x$ catalyst for Methanol steam reforming produces H_2 gas with yield of 87.5%.

Poster Presentation : **INOR.P-225**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Helical Fluxionality of Tricopper Cluster Complex

Heechan Kim, Dongwhan Lee[*]

Department of Chemistry, Seoul National University, Korea

We present a trinuclear copper(I) complex that exhibits helical motions for intramolecular site exchange. A pentadentate ligand L was designed to support multiple metal centers. Strategic placement of sterically demanding groups along the π-conjugated backbone facilitated the formation of a helical assembly upon metal binding. X-ray structure of the resulting complex $[Cu_3L_2]^{2+}$ revealed the C_2-symmetric metallohelicate core held by tight intramolecular π–π contacts. With the *N*-donor atoms closely positioned along the rigid ligand backbone, the helicate features short Cu–Cu distance of ca. 2.8 Å. Intriguingly, the ^{1}H NMR spectra of $[Cu_3L_2][BF_4]_3$ show highly symmetric resonance patterns in polar solvents, whereas a lower symmetry is observed in nonpolar solvents that is consistent with the solid-state structure. Variable-temperature (VT) ^{1}H NMR spectroscopic studies revealed that the metallohelicate undergoes rapid intramolecular ligand substitution reactions to allow thermoneutral site-exchange of three copper(I) ions hoping back and forth inside the helical cavity carved out by ten *N*-donor atoms. This presentation will discuss the underlying mechanism of this hitherto unknown helical fluxionality of cluster complex.

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Poster Presentation : **INOR.P-226**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Study on Gas Sorption behavior in the functionalized Hydrogen bonded Porous Coordination Polymer(HPCP)

Jong Won Shin[*], **Dohyun Moon**[1,*]

Division of Daegu, Korea Institute of Science and Technology Information, Korea
[1]*Beam Operation Team, Pohang Accelerator Laboratory, Korea*

Although great development and progress have been made in design, synthesis, characterization, and performance expansion of MOFs or PCPs, new MOFs or PCPs material with stable structure properties related with water, thermal and solvent, still need to explored further. Recently, PCPs or MOFs formed by intra-/inter-molecular interactions (e.g. hydrogen bond and π- π interaction) have been attracted much attention from chemist, material scientist, especially strong hydrogen bonded porous coordination polymer (HPCP) formed by connecting various dimension (zero, 1-D, 2-D) back bond or building blocks.Recently, a HPCP Ni(II) complex, $[(BTB)_2Ni_3((C_{16}H_{38}N_6)_3(H_2O)_4]$•guest (**1**) , was synthesized by the self-assembly of Ni(II) azamacrocyclic backbone with H_3BTB(1,3,5-Tris(4-carboxyphenyl)benzene ligand. In **1**, the coordinated water molecules of Ni(II) azamacrocyclic form strong intermolecular hydrogen bonds with adjacent BTB ligand and stabilize the molecular structure and give rise to a strong 3-D hydrogen-bond HPCP.Although the compound 1 possessed poor porosity by void volume and N_2 sorption, **1** showed significant isotherms for several gases (*i*.e. CO_2, C_2H_2, .CH_4) with hysteresis and gate opening at 196 K. Here, we will explain the crystal structure, PXRD with gas, sorption properties as well as interesting coordination chemistry.

Poster Presentation : **INOR.P-227**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of gold-silver bimetallic nanowires for efficient electrochemical CO_2 reduction

Jonghyeok Park, Hyunjoon Song*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The increase of the concentration of carbon dioxide due to the usage of fossil fuels causes global warming that affects critical influence. Electrochemical CO_2 reduction reaction (eCO_2RR) was suggested as a solution to decrease the CO_2 concentration. CO, one of the major products of eCO_2RR, is a favorable product from eCO_2RR due to its wide usage such as the Fischer-Tropsch reaction. For CO production, Ag showed a promising result with high selectivity. Ag nanocatalysts were synthesized to increase selectivity with various morphologies, facets, and sizes. The nanowire, one of the 1D structures, was chosen for CO_2 reduction due to its high stability for electrochemistry. Through the polyol methods, 5-twinned Ag nanowires were synthesized. Bimetallic nanocatalysts can increase CO selectivity by controlling metal properties. Au was applied to Ag nanowires by galvanic replacement reaction to decrease the high overpotential of Ag for eCO_2RR. By testing electrochemical CO_2 reduction of Ag and AuAg nanowires in H-cell, Ag and AuAg nanowires convert CO_2 to CO with faradaic efficiency of 75% and 96% at -1.05 V and -0.85 V versus reversible hydrogen electrode, respectively.

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Poster Presentation : **INOR.P-228**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Kinetically Controlled Supramolecular polymeric nanosheets based on rearranged Zinc porphyrin complexes in aqueous media

Sukyoung Kim, Jong Hwa Jung*, Sung Ho Jung*

Department of Chemistry, Gyeongsang National University, Korea

Despite its great potential in supramolecular chemistry to achieve structural complexity and sophisticated functionality, the kinetic control over the molecular self-assembly in coordination supramolecular polymerization still constitutes a challenge. Herein, I report the metalation-dependent assembling behavior shown by porphyrin derivative, which formed different supramolecular polymers with/without Zinc ions in aqueous media, that is, H-aggregation (nanoparticles) and J-aggregation (nanosheet with Zn), respectively. The distinct porphyrin cores of $\mathbf{1}_{\mathbf{free}}$ and $\mathbf{1}_{\mathbf{Zn}}$ undergo different aggregation pathways. In the presence of Zn(II) ions, the H-type aggregation formed by $\mathbf{1}_{\mathbf{free}}$ is in metastable state, and the synthesis of monomeric $\mathbf{1}_{\mathbf{Zn}}$ via metalation retards the spontaneous J-aggregation. The seeding method was successfully applied to produce two-dimensional nanosheets in the present of Zn(II) ions. This kinetically controlled metalation provides a platform for the development of supramolecular metal-based structures with controlled size, morphology, and chemical properties. I believe that the present metal insertion-based complexation approach will contribute to further advances in the field of living supramolecular polymerization and its applications.

Poster Presentation : **INOR.P-229**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

The formation and characteristics of the seeded living supramolecular polymerization of Tb(III) complexes with terpyridine-based ligand

Minkyeong Hwang, Jong Hwa Jung[1,*]

chemistry, Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*

The seeded living supramolecular polymerization was synthesized using Tb(III) complex. After supramolecular polymerization of Tb(III) complex with terpyridine ligand. The seed (Tb-$\mathbf{1}_{seed}$) of supramolecular polymer, Tb(III) complex was prepared by ultrasonication at 10℃. SEM images showed 250-300 nm of lengths with a narrow polydispersity. After multicycles in seeded living supramolecular polymerization, the lengths of polymers increased gradually. These results indicate that the living supramolecular polymerization occurred at active termini of seed. The formation of supramolecular polymers was also analyzed using UV/Vis spectroscopy, fluorescence spectroscopy, scanning electron microscopy (SEM), and dynamic light scattering method (DLS). In this meeting, we will present on the synthesize of seeded living supramolecular polymerization in detail.

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Poster Presentation : **INOR.P-230**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Preparation of supramolecular polymer based on Eu(III) complex by seeded living polymerization

Seol A Lim, Jong Hwa Jung[1,*]

chemistry, GYEONGSANG NATIONAL UNIVERSITY, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*

The seeded living supramolecular polymerization was synthesized using Eu(III) complex. After supramolecular polymerization of Ag^+ complex with terpyridine ligand, The seed ($\text{Eu-}\mathbf{1}_{\text{seed}}$) of supramolecular polymer based on Eu(III) complex was prepared by ultrasonication at 10 °C. SEM images showed 250-300 nm of lengths and a narrow polydispersity (PDI = 1.05). After multicycles by seeded living supramolecular polymerization, the lengths of polymers increased without PDI. These results indicate that the living supramolecular polymerization occurred at active termini of seed. The formation of supramolecular polymers was characterized using UV/Vis spectroscopy, fluorescence spectroscopy, scanning electron microscopy (SEM), and dynamic light scattering method (DLS). In this meeting, we will present on the synthesize of seeded living supramolecular polymerization in detail.

Poster Presentation : **INOR.P-231**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Kinetically controlled Pt(II) complex-based supramolecular polymers by exchange of ligand

Minhye Kim, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

We prepared square planar Pt(II) complex by terpyridine ligand and $PtCl_2$. The tri-nitrogen atoms of terpyridine moiety and one chloride anion were coordinated to Pt(II) ion. To exchange chloride ion into pyridine, the pyridine was added to Pt(II) complex in DMSO and water. The solution was observed photoluminescence (PL) spectral changes by PL spectrophotometer. It was confirmed that the PL emission at 610 nm was shifted to 570 nm. The PL emission at 570 nm was returned to original position upon addition of HCl. In addition, supramolecular polymerization process was determined by UV-vis spectrophotometer. As the result, the polymerization follows on-pathway. The thermodynamic parameters of supramolecular polymers were determined from heating curve using global fitting program. In this annual meeting, we will discuss on the formation of supramolecular polymers based on Pt(II) complex and their thermodynamic parameters in detail.

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Poster Presentation : **INOR.P-232**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Ag^+supramolecular polymers induced by change of conformation in the alkyl chain

Hyeon Min Han, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Two terpyridine-based ligands possessing trans or cis double bonds in the alkyl chain were synthesized by several steps. These ligands formed silver(I) complex in water. The stoichiometric ratio of Ag^+ complex was characterized by ESI mass spectroscopy. Supramolecular coordination polymers formed by Ag^+ showed the strong circular dichroism (CD) signals in a mixture of H_2O and dimethyl sulfoxide (DMSO). The strong positive CD signals of supramolecular polymers were obtained upon addition of $AgNO_3$ (1.0 equiv.), indicative of right-handed helicity. In contrast, the negative CD signal of ligand possessing trans-double bond in the alkyl chain, was observed in the presence of 0.5 equiv. of $AgNO_3$, indicating the supramolecular polymers have left-handed helicity. SEM images of supramolecular polymers showed the fiber structure. In this annual meeting, we will discuss on the formation of supramolecular polymers in the presence of $AgNO_3$.

Poster Presentation : **INOR.P-233**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Chiral Supramolecular Nanostructure Based on Pt(II) Complexes

Chenxing Li, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Supramolecular Nanostructure have great potential for biomedical applications because of their sensitivity to a variety of biological stimuli, their rapid biodegradation, and the ease with which they can be incorporated into bioactive components. Terpyridine is used as one of the typical ligands in transition metal catalysts due to the low LUMO and geometric/steric advantages of its pyridine ring, which enhance the stability and reactivity of transition metal centers. Thus, we synthesized three Pt(II) complexes with terpyridine ligands by multi-steps. The synthesized Pt(II) complexes were characterized by ^{1}H, ^{13}C NMR, FT IR and ESI mass spectrometers. In addition, the helical properties of supramolecular polymers based on Pt(II) complexes were demonstrated by circular dichroism (CD) spectroscopy. The strong negative CD signals were observed at 550 nm, which originated from Pt-Pt interaction. In this annual meeting, we will present on chiral supramolecular polymerization in detail.

Poster Presentation : **INOR.P-234**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Mono- and Dinuclear Zinc Complexes Bearing Identical Bis(thiosemicarbazone) Ligand that Exhibit Alkaline Phosphatase-like Catalytic Reactivity

Hyeri Jeon, Hyungbin Park[1], Chaewon Ahn, Seungwoo Hong*

Department of Chemistry, Sookmyung Women's University, Korea
[1]*Sookmyung Women's University, Korea*

Mono- and dinuclear zinc(II) complexes bearing bis(thiosemicarbazone) (bTSC) ligand were employed in the cleavage of phosphoester bonds. Comparative kinetic studies combined with theory suggested that the P–O bond cleavage is much accelerated by dinuclear zinc(II) complex in the presence of base. Based on the DFT-optimized structures of the proposed intermediates, it is plausible that (**1**) the removal of sulfur atoms of bTSC ligand from the zinc center provides two vacant sites for the binding of water (or hydroxide ion) and phosphoester and (**2**) the H-bonding between water (or hydroxide ion) and phosphoester, through several water molecules, may also assist the P–O bond cleavage and facilitate the nucleophilic attack. The kinetic and catalytic studies on the hydrolysis of phosphoester by dinuclear zinc complex showed a much enhanced reactivity under basic reaction conditions, reaching over 95% conversion yield within 4 h. The currently presented compounds are arguably one of the faster synthetic Zn-based model performing phosphatase-like activity presented so far.

Poster Presentation : **INOR.P-235**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

A Nonheme Ferrous Model Complex Driven Ferroptosis-Like Cell Death in Renal Cancer

Hyungbin Park, Hyeri Jeon[1], Chaewon Ahn[1], Seungwoo Hong[1,*]

Department of Chemisry , Sookmyung Women's University, Korea

[1]*Department of Chemistry, Sookmyung Women's University, Korea*

Cancer is one of the leading causes of morbidity and mortality in the world, but more cancer chemotherapies are needed to complement existing regimens due to problems of existing cancer chemotherapies such as aggressive side-effect and drug resistance.While apoptosis has long dominated the spotlight in the past two decades and have expanded the repertoire of programmed cell death (PCD), ferroptosis, a new type of cell death discovered in recent years, is an emerging pathway of cancer cell death. Ferroptosis is usually accompanied by a large amount of iron accumulation and lipid peroxidation during the cell death process; the occurrence of ferroptosis is iron-dependent. Herein, we synthesized nonheme metal complexes bearing HN5O ligand (2-((2-(bis(pyridin-2-ylmethyl)amino)ethyl)(pyridin-2-ylmethyl)amino)ethanol). They were characterized by various spectroscopic techniques such as UV−vis spectroscopy, cyclic voltammetry, nuclear magnetic resonance (NMR) and electrospray ionization mass (ESI-MS). We confirmed that the H2O2 activation by iron complex was occurred via Fenton-like reaction and hydroxyl radical was quantitatively generated. Renal cell carcinoma (RCC), also known as renal cell cancer or renal cell adenocarcinoma, is the most common type of kidney cancer. When the iron complex incubated in renal cancer cells (Caki-1, A498, 786-O), it has ability to induce ferroptosis by catalyzing Fenton-like reaction in cancer cells; higher concentrations of ROS in intracellular networks lead to ferroptosis.

Poster Presentation : **INOR.P-236**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Selective Formation of Multinuclear Iridium Supramolecules by using Tetrazolyl Ligands

Guitae Park, Junseong Lee[1,*]

chemistry, Chonnam National University, Korea

[1]*Department of Chemistry, Chonnam National University, Korea*

In the self-assembly of supramolecules, it is very important to control the shape and them and nucleari-ty of metal centers simply for the further applications such as catalysis and magnetism study. For the precise control of nuclearity of Ir metal center, several synthetic strategies could be considered as follows: (i) making additional bind-ing site in the metal center by removing chloride ion (ii) opening or blocking nitrogen site of tetrazolyl part (iii) modulating connection angle by controlling chelating mode. With these concepts, we tried to control the nuclearity of Ir metal centers. In addition, we describe the selective synthesis of multinuclear iridium supramolecules having different shapes by means of the binding mode control of tetrazole ligands. By controlling the reaction condition, different ligations of tetrazolyl lig-ands were achieved. In this article, we report the selective synthesis of mono-, di-, tetra- and hexa-nuclear half sandwich iridium supra-molecules containing chelating tetrazolyl units for new irid-ium hetermetallic assemblies.

Poster Presentation : **INOR.P-237**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Radon Concentration in Groundwater of Jeju Island

Sohyeon Lim, Chung-Hun Han, Hee-Jung Im*

Department of Chemistry, Jeju National University, Korea

In the present study, radon (222Rn) concentrations in groundwater in Jeju Island were performed by using RAD H2O of RAD7. Groundwater samples were collected from 10 sites from March to April 2022. The activities of 222Rn in groundwater were in the range of 0 to 60 Bq L−1. The radon mean concentration in Jeju was in the order of Southern > Northern > Western > Eastern region. There was no groundwater exceeding the range of 148 Bq L−1 proposed by the US EPA guideline value. The effective dose from radon due to intake of drinking water is less than the recommended value of 100 µSv y−1.

Poster Presentation : **INOR.P-238**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of a surfactant free Rhenium Oxide Nanocube and their photocatalytic performance

Kang min Lee, Seok Min Yoon[1,*]

Department of chemistry, Wonkwang University, Korea
[1]*Department of Chemistry, Wonkwang University, Korea*

Most nanomaterials synthesis by wet-chemistry have required surfantant, but the coated surfant on their surface possibly hinder electron transfer decresing efficiency of catalysis. Therefore, we synthesized mixed-valence rhenium oxide (MV-ReOx) nanocubes by the solvothermal method without any surfactant. Thus, we compared photocatalytic activity with surfactant coated MV-ReOx nanoparticles, surfactant-free MV-ReOx nanocubes and P25 $TiO2$ photocatalysts for dissociation of organic dye molecule like methyl-orange. Under visible light irradiation, interestingly, the surfactant-free MV-ReOx showed most effectively dessociating such organic pollutant by photocatasltic effect. The results imply that the surfactant-free MV-ReOx cubes can be efficient photocatlyst, and applicable for other photocatalytic systems such as photo-water splitting and artificial synthesis and so on.

Poster Presentation : **INOR.P-239**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Reconstruction Pathway of Bismuth Oxyiodide: Dependence on Crystal Structure, Electrocatalytic CO_2 Reduction

Taewaen Lim, Junhyeok Seo[*]

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Fossil fuel-based energy system and inevitable CO_2 emission are thought of being causative of the current climate issues. Research efforts to discover methods for utilizing the gas would be helpful to delay the drastic climate changes. Electrochemical reduction is one of the promising methods for utilization of CO_2 due to the relatively simple reaction scheme. Nonetheless, the high potential energy and low product selectivity have remained challenging in the research of developing electrocatalysts. Bismuth-based materials have received spotlights because of the selective activity for the CO_2-to-formate reduction. Recent studies revealed that complicated chemical reactions, such as reconstruction and dismantling, generally occur in the working conditions using bismuth-containing electrocatalysts. Herein, we study the electrochemical reactivity of bismuth oxyiodide (BiOI) nanosheets and the crystalline structure-dependent reactivity. BiOI nanosheet showed a phase transition reactivity from tetragonal to orthorhombic. The varied crystalline phases were tested for the electrocatalytic CO_2 reduction. We could observe the highly efficient CO_2-to-formate conversion up to 95 % at the low potential of -0.86 V versus reversible hydrogen electrode. In this poster, we will discuss 1) crystalline phase transition of BiOI nanosheet, 2) reactivity of BiOI nanosheet with electrolytes, and 3) electrocatalytic CO_2 reduction to formate.

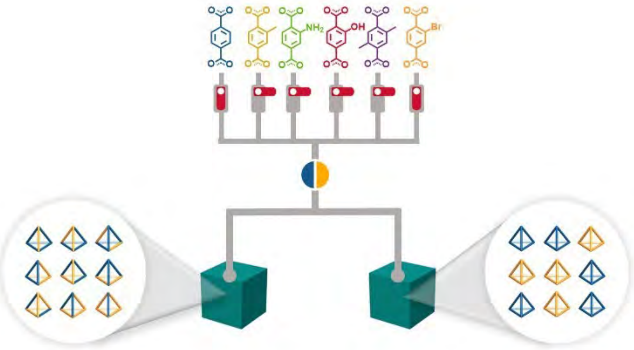
Poster Presentation : **INOR.P-240**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Self-Assembly Beyond Randomness: Multivariate Porous Platform Based on Metal-Organic Polyhedra

Dongsik Nam, Jiyeon Kim[1], Joohan Nam, Tae-Hyuk Kwon[*], Wonyoung Choe[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Chemistry, Ulsan National Institute of Science and Technology, Korea*

Porous solids with multiple functional groups mixed in periodic backbones, i.e., multivariate porous solids, have become a fascinating material platform for a broad range of applications due to emerging properties apart from single-component counterparts. Thanks to reticular chemistry, metal-organic frameworks (MOFs) became such a platform material targeting versatile applications. However, little is known about how various functionalities are assembled at the molecular level because multivariate solids have been realized in extended frameworks. Controlling the functionality assembly is a further challenge. We envision that frameworks composed of discrete cages can be a breakthrough material with molecular-level control using the solubility of the cages. Here we present a unique multivariate platform based on metal-organic polyhedra (MOPs). The MOP platform allows discovering cage populations in the backbone structure and controlling the assembly of functional groups that were significantly hampered in a typical MOF platform. We expect the emergence of such a cage-based multivariate platform will have a great impact on the development of fascinating applications using porous molecular solids.Reference: D. Nam et al. *Matter* **2021**, *4*, 2460–2473.


NH2
OH
Br

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Poster Presentation : **INOR.P-241**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Reducing V_{OC} loss in perovskite solar cell with novel cathode interfacial layer

Jihyun Min, Sangah Park[1], Taiho Park[2,*]

chemical engineering, Pohang University of Science and Technology, Korea
[1]*Chemical Engineering, Pohang University of Science and Technology, Korea*
[2]*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*

The interfacial layer has contributed a lot to the development of perovskite solar cells (PSCs). In perovskite solar cells, the interfacial layer shifts the energy levels, attracts and extracts charges and passivates surface traps, resulting in improving both efficiency and stability of the PSCs. Herein, we report a small molecular self-assembled monolayer (2-[carbamimidoyl(methyl)amino]acetic acid), which is called creatine as a interfacial layer between perovskite and SnO_2 layer. Creatine is anchored to the SnO_2 layer due to its structural properties. It enhances charge extraction from the perovskite layer by forming dipoles at the interface and reducing the work function. In addition, creatine also reduces defect density by passivating many defects present at the perovskite interface. As a result, the formamidinium-based PSCs introducing creatine layer achieves the highest power conversion efficiency (PCE) of 22.1%.

Poster Presentation : **INOR.P-242**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Topology-Guided Roadmap for Reticular Chemistry of Metal-Organic Polyhedra

Jiyeon Kim, Wonyoung Choe[1,*]

Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Topological considerations for linking building blocks, namely reticular chemistry, have played a central role in designing new structures, as widely applied for extended material platform, metal-organic frameworks (MOFs). After witnessing the successful case of MOFs, we envisioned the extension of reticular chemistry to molecular solids built from much different interactions, such as hydrogen bonds and electrostatic interactions. We have identified a new subclass of metal-organic materials, where the principle of reticular chemistry can be applied, despite the absence of strong coordination bonds. Zr-based metal-organic polyhedra (MOPs) are notable examples. In this presentation, we propose an extension of reticular chemistry by revealing how topology is involved in cage assembly and showing how topology can be utilized to discover future structures of Zr-based MOPs (Figure 1). We expect that the reticular chemistry of Zr-based MOPs will serve as a blueprint for building future MOPs. Topological insight for decoding packing structures opens new avenues for enriching the repertoire of reticular chemistry pertaining to cage-based frameworks.Reference:Kim, J.; Choe, W. Chem 2022, accepted. DOI: 10.1016/j.chempr.2022.02.008.

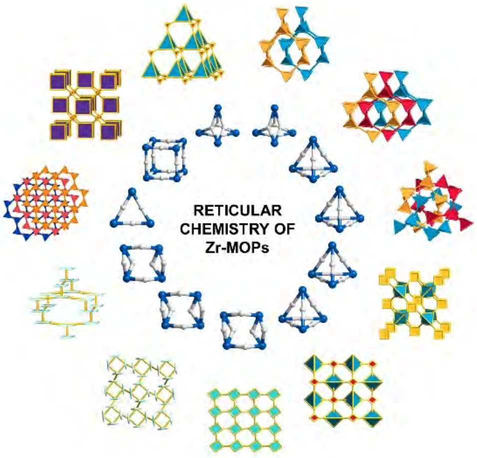

Figure 1. Decoded packing structures of Zr-based metal-organic polyhedra.

Poster Presentation : **INOR.P-243**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Realization of SiN_x nanofilters using nanoimprint lithography for synthesis of green Cs_3MnBr_5 phosphors

Minji Ko, Hyengjin Kim[1], Keyong Nam Lee, Young rag Do[2,*]

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[2]*Department of Bionano Chemistry, Kookmin University, Korea*

In this study, we used SiN_x nanofilters to synthesize green Cs_3MnBr_5 phosphors through purification of reactant solutions. To fabricate the SiNx nanofilters, nanopore patterns were successfully fabricated on 6-inch Si wafer via nanoimprint lithography. We next optimized the fabrication process of SiN_x nanofilters though dry and wet etching. The reactant solutions for green Cs_3MnBr_5 were filtered using a fluidic device with built-in SiN_x nanofilters. The filtered reactant solutions were synthesized through evaporative crystallization. To improve photoluminescence quantum yield (PLQY), the reactant solutions were filtered by controlling the pore sizes of the SiN_x nanofilters from 50 nm to 200 nm by coating with Al_2O_3. The PLQY of the purified green Cs_3MnBr_5 phosphors filtered by 50 nm-nanohole arrayed SiN_x nanofilter was found to be 2.3 times higher than that of the non-filtrated green Cs_3MnBr_5 phosphors due to the removal the unnecessary residual nano-particles in reactant solutions. The highest PLQY of the purified green Cs_3MnBr_5 phosphors was 51%. The peak wavelength and full-width at half-maximum (FWHM) of emission spectra were 524 nm and 40 nm, respectively. Therefore, SiN_x nanofilters using nanoimprint lithography have potential for application to chemical purification, biological purification, and other applications.

Poster Presentation : **INOR.P-244**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Re-Pt-Ni tertiary alloy nanoparticle cluster as a highly efficient hydrogen evolution electrocatalyst under the entire pH range

Jinho Kim, Seok Min Yoon[1,*]

Department of chemistry, Wonkwang University, Korea
[1]*Department of Chemistry, Wonkwang University, Korea*

The world's energy demand has increased rapidly and continuously over the past few decades. Developing sustainable and eco-friendly future energy is the biggest challenge we need to solve now. Hydrogen is a clean energy source that has received a lot of attention. The hydrogen evolution reaction (HER) produces molecular hydrogen through the electrochemical reduction in water. Efficient HER electrocatalysts must meet various conditions such as low overpotential, high stability, and low cost. The most effective electrocatalyst for HER is platinum (Pt)-based catalysts, but they are expensive. Therefore, HER has been comprehensively studied for several metals. However, few studies have examined the rhenium (Re)-based electrocatalyst activity for HER, although Re has a much lower price than Pt. The volcano plot shows that rhenium has an exchange current density comparable to that of Pt and has adequate binding energy for proton adsorption and desorption. Herein, we present a very effective electrocatalyst for HER catalyst, a Re-based tertiary alloy nanoparticle cluster containing a tiny amount of Ni and Pt aggregated with amorphous carbon (a-C). In alkaline conditions, HER is known to hinder the development of water-splitting techniques for high-purity hydrogen production because it involves a slow water dissociation process. Nevertheless, the Re-based nanoparticle cluster catalyst performed lower overpotential and higher stability than Pt under alkaline conditions. In addition, it shows performance similar to Pt under acidic conditions. These nanocomposites are a novel candidate to replace Pt catalysts for electrochemical HER, which are now commercially available to be applied in industrial hydrogen production.

Poster Presentation : **INOR.P-245**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Stable Cu(I) Complexes by New Bisquinoline Schiff Base Ligand

Eun su Chae, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Copper complexes are mostly stable at Cu(II) state, and unstable at Cu(I) state. For this reason, many studies of catalytic reaction by using copper complex mainly focused in oxidation process.However, there has few studies of catalytic reaction by using stable Cu(I) complex which focused in reduction process. These reduction process has high reduction potential which can reduct highly stable compounds like carbon dioxide.In this study, we have synthesized new bisquinoline schiff base ligand EbQMA (=(N*E*,N'*E*)-2,2'-(ethane-1,2-diyl)bis(N-(quinolin-8-ylmethylene)aniline)) and stable Cu (I) complexes, [Cu(EbQMA)]ClO_4 and [Cu_2(EbQMA)I_2]. These copper complexes were monitored by NMR spectroscopy and SCXRD analysis.

Poster Presentation : **INOR.P-246**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Electrical Conductivity and Tunable Photoluminescence of Halogen Doped Lithium perrhenate crystal

Sojeong Lee, Seok Min Yoon*

Department of Chemistry, Wonkwang University, Korea

Lithium perrhenate (LiReO4) can be one of the electrochemical energy storage materials owing to incorporated Li metals in their crystal structure. Up to date, the synthetic protocol of lithium perrhenate is required high temperature and multiple synthetic steps. However, we developed a one-pot synthetic method to produce lithium perrhenate lower than 100℃. We successfully synthesized LiReO4 by simply mixing lithium salts consisting of halogens (X: F, Cl, Br, I) with Re2O7 in aqueous media. Further, we found the synthesized LiReO4 has a mixed-valence oxidation state of Re (Re7+ and Re6+), and their crystalline material is doped with halogens. Owing to their mixed-valence oxidation state and halogen doping effect, the synthesized LiReO4 (X-LiReO4 (X: F, Cl, Br, I)) exhibit high electrical conductivity up to 4.86 S cm-1, which is Iodine doped one. Moreover, the synthesized LiReO4 showed tunable photoluminescence (PL) in the Near-IR range (750 nm ~ 850 nm) depending on the excitation wavelength, while intrinsic LiReO4 (not doped and no mixed-valence oxidation state) did not exhibit PL and they are almost insulator.

Poster Presentation : **INOR.P-247**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Eco-friendly and Stable I-III-VI Quantum Dots embedded Al_2O_3 microbeads using electrospraying

Eunha Hong, Minji Ko, Yun Jae Eo, Hyeongjin Lee[1], Young rag Do[2,*]

Department of Chemistry, Kookmin University, Korea

[1]*Department of Applied Chemistry, Kookmin University, Korea*

[2]*Department of Bionano Chemistry, Kookmin University, Korea*

Recently, broadly emissive I-III-VI quantum dots (QDs) such as Cu-In-Zn-S and Cu-Ga-Zn-S have been studied as alternatives to toxic Cd- and Pb-based QDs used in optoelectronic devices. Using a concerted synthetic process of e-spraying and fast hydrolysis, broadband green and red emissive I-III-VI QD-embedded Al_2O_3 (QD@Al_2O_3) microbeads are synthesized as an efficient, stable and easy-to-use QD material form to be applied to down-converting white light-emitting diodes (DC-WLEDs). An aluminum tri-sec-butoxide ($Al(O\text{-}sec\text{-}Bu)_3$) solution was selected as a fast hydrolysis precursor containing QDs to fabricate a spherical form of QD@Al_2O_3 composite powders during the e-spray process. The photoluminescence quantum yields (PLQYs) of the resultant green $Zr(PrO)_4$-CuGaZnS/ZnS and red $Zr(PrO)_4$-CuInZnS/ZnS QD solutions were 94.5% and 95%, respectively. Their PLQY and operational stability were improved by reducing the ligand loss via passivation and encapsulation role of the $Zr(PrO)_4$ complex over the QD surface in $Zr(PrO)_4$-treated QD@Al_2O_3 powders. A WLED single package implemented with GR $Zr(PrO)_4$-treated QD@Al_2O_3 microbeads showed comparable luminous efficacy (LE = 77.0 lm/W) with a high color rendering index (> 92). The LE of a WLED with $Zr(PrO)_4$-QD@Al_2O_3 microbeads was improved by 41% compared to that of a WLED with pristine QD@Al_2O_3 microbeads. We also realized temporal progress in relative LE stability tests of green and red QD@Al_2O_3 microbead films during an applied time of 72 hr at 60 mA. The e-spray hydrolysis process of QDs and a reactive metal alkoxide solution provides a simple and novel synthetic platform process to produce easy-to-use spherical QD-embedded solid materials for PL-DC applications into future QD-based lightings and displays.

Poster Presentation : **INOR.P-248**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Nanographene-based Metal-Organic Frameworks

Junghye Lee, Young S. Park*, Wonyoung Choe*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Nanographene with extended π-conjugated structures has been attracted synthetic interest with great potential in photophysical and electrochemical properties. However, most nanographene fragments show self-assembled utilize their strong π-π interaction so that the resulting structures barely possess any open π surface. In this context, metal-organic frameworks (MOFs) have uniform cavities and highly ordered arrays in the structure. Thus, MOF can serve the isolate large π-conjugated surface into periodic arrays by avoiding the π-π interaction.In this work, we successfully obtained nanographene-based MOFs utilizing the hexatopic organic linkers, hexabenzocoronene (HBC) and hexaphenylbenzene (HPB). We also adjusted the pore environment by changing the linker content of the MOF structure. Nanographene MOFs reported in this poster will be used as the removal of polycyclic aromatic hydrocarbons (PAHs) and photocatalyst.

Poster Presentation : **INOR.P-249**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Diphiylleia grayi-inspired hydrochromic PDMS film using nanosphere lithography

SeungJe Lee, Hyengjin Kim[1], Selim Yun, Young rag Do[2,*]

Kookmin University, Korea
[1]*applied chemistry, Kookmin University, Korea*
[2]*Department of Bionano Chemistry, Kookmin University, Korea*

Diphiylleia grayi are mysterious flowers that become transparent on rainy days. We inspired the hydrochromic properties of these flowers and fabricated a smart film that becomes transparent when wet state. *Diphiylleia grayi*-inspired hydrochromic film was fabricated by forming a nanocavity structure on the surface of a Polydimethylsiloxane (PMDS) film. These hydrochromic film, fabricated by nanosphere transfer methods, were optimized using various size of polystyrene bead (200, 400, 600, 1,000, 2,000 nm). These nano cavity structure was fabricated by a combination of polystyrene (PS)-based nano-sphere lithography (NSL) and PDMS transfer method. Nanosphere lithography using polystyrene bead have the several advantage of easily adjusting the diameter to obtain a variety of nano structure and inexpensive process. Among them, the 1,000nm cavity structure PDMS film showed the greatest contrast between the wet and dry state. (44.93% (ΔTD) T = 59.11–14.18%) and 54.88% (ΔH = 69.42–14.54%). Due to the largest contrast ratio, it can be applied to various hydrochromic application that require color change such as smart window, camouflage, and transparent umbrellas on rainy days. To achieve wettability, we performed a surface modification using polyvinyl alcohol (PVA). The PDMS film surface was measured by scanning electron microscope (SEM). The scattering effect of nano cavity structures was measured by UV-visible spectroscopy and haze value measured using by hazemeter.

Poster Presentation : **INOR.P-250**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

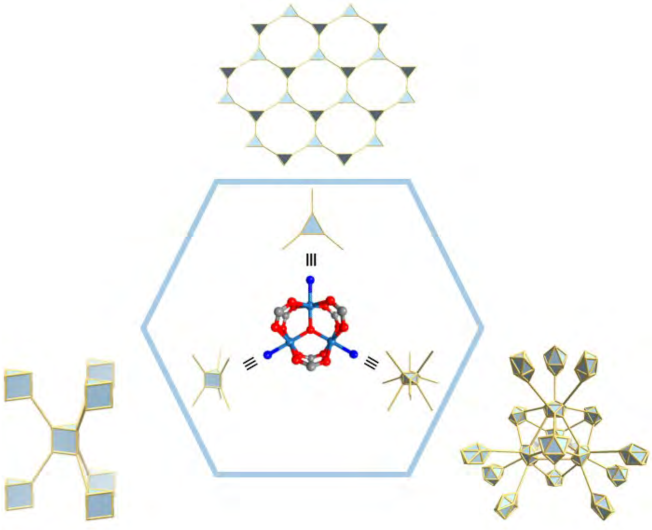
Multivariate Analysis of Metal-Organic Frameworks with M3O Secondary Building Units

Eunchan Jo, Wonyoung Choe[1,*]

Ulsan National Institute of Science and Technology, Korea

[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

The secondary building unit (SBU) approach is a turning point in the discovery and design of metal-organic frameworks (MOFs). When using an SBU with multiple connectivity, more diverse topologies can be created with just one cluster. M3O is a well-known SBU capable of simultaneously having 3-connectivity (3-c), 6-c, and 9-c. Although versatile structures synthesized using M3O have been reported experimentally, a comprehensive study on the structures that can be built from SBUs with multiple connectivity is in its infancy. In this presentation, we provide future structures that can be designed from M3O with multiple connectivity through topology analysis. We expect that this topological study can accelerate the emergence of new MOF structures.



Poster Presentation : **INOR.P-251**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Spatial local Heterogeneity Have Effect on the Unusual Uptake Behavior of MTV-MOFs.

Soyeon Ko, Kyungmin Choi*

Chemical and Biological Engineering, Sookmyung Women's University, Korea

The unique adsorption properties in MTV-MOFs have been deciphered by apportionments of multiple functional groups existing all over the crystals, which is one of the key factor to discover unknown opportunities of MTV-MOFs. In the extension of the apportionment type, we hypothesized that the spatial locality of the apportionment would affect on the unique sorption behavior and unveil an important factor contributing to MTV-MOFs. In this study, we chose BDC-H (1,4-benzenedicarboxylate, indicates as A) and BDC-NH2 (2-amino-1,4 benzenedicarboxylate, indicates as B) linkers to give affinity difference to absorbent, then prepared three types of MOFs to elucidate the decisive role of spatial locality in MTV-MOFs: (1) MTV-MOF-AB adopting UiO-66 structure containing BDC and BDC-NH2 linkers all over the crystals , (2) MTV-MOF-A⊂B having BDC-NH2 linker outer part and BDC-H linker inner part of its particles , (3) MTV-MOF-B⊂A having BDC-H linker outer part and BDC-NH2 linker inner part of its particles . Interestingly, the CO2 uptake behavior of MTV-MOF-A⊂B was like that of MOF-B while that of MTV-MOF-B⊂A was like that of MOF-A. It was also found that H2O sorption at 298 K showed similar behaviors. These evidence of CO2 and H2O uptake lends support that the sorption behavior of MTV-MOF-AB was highly affected by specific functionality of outer part of its crystal. These findings were also supported by visualization of iodine sorption using transmission electron electroscopy (TEM).

Poster Presentation : **INOR.P-252**

Inorganic Chemistry

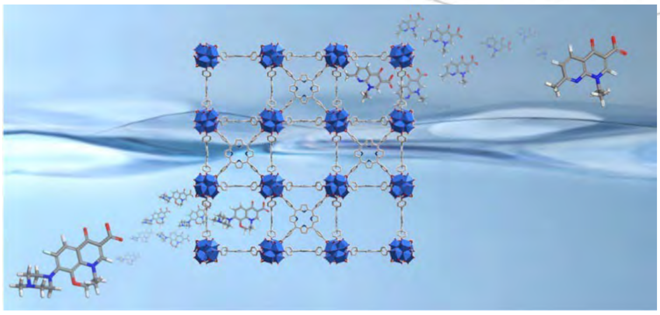
Event Hall FRI 11:00~13:00

Interaction of drug and dye molecules with Zr-clusters: DFT studies in the implicit solvent model

David Yang, Eunyoung Kang, Eunji Jin[1], Jiyeon Kim[2], Joohan Nam, Wonyoung Choe*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany*
[2]*Chemistry, Ulsan National Institute of Science and Technology, Korea*

Absorptive removal of organic contaminants from water has been met with difficulties such as high cost, byproduct formation, and complicated processibility. We present the Zr-based metal-organic framework PCN-224 as an absorptive material with several desirable properties for this purpose, such as high surface area, good water stability, and pore controllability. In particular, we use density functional theory calculations to show how the energetic favorability of coordinate bonding of some selected molecules (methyl orange, nalidixic acid, ofloxacin, naproxen, and ibuprofen) with the highly valent Zr in the nodes of PCN-224 is a property that can be generally assumed for other MOFs with similar composition and structural properties. Our findings contribute to the advancement of MOF design and synthesis and provide a new direction for the adsorptive removal of harmful molecules from from water.



Poster Presentation : **INOR.P-253**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Structural modification from MIL-101 to MIL-53 by water addition

Mingyu Gu, Cheongwon Bae, Juyeong Kim*

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Korea

Trace substances are critical in terms of obtaining a targeted structure in the synthesis of metal–organic frameworks (MOFs). Herein, we investigated an influence of water to the crystal structure of Fe-based MIL-101. As the water content increased from 0 to 1.0 wt%, the product structure transformed from MIL-101 to MIL-53. Also, iron oxide nanoparticles began to form on the surface of the MIL nanoparticles, confirmed by scanning electron microscopy. The product synthesized with different water content was further examined using infrared spectroscopy, thermogravimetric analysis, and Brunauer-Emmett-Teller surface area analysis.

Poster Presentation : **INOR.P-254**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Structure-direction and Phase Transformation toward Porous Zeolitic Imidazolate Frameworks

Soochan Lee, Wonyoung Choe*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Solvothermal synthesis is the most common synthetic method to grow the crystals of metal-organic frameworks (MOFs). The synthetic condition for desired MOF crystals should be considered with the combination of thermodynamic and kinetic factors. However, controlling these factors is extremely difficult to predict all stages of the reaction coordinate. Zeolitic imidazolate frameworks (ZIFs) are zeolite-mimic MOFs from coordination bonds between four-coordinated transition metals and various imidazolate (Im) linkers. Bulky functional groups in Im derivatives afforded the porous ZIFs via structure-direction of functional groups. However, ZIFs with only basic Im (no functional groups, $Zn(Im)_2$) exhibited dense phase polymorphs because of the absence of structure-direction. This presentation suggests the new synthetic method to obtain the porous phase of $Zn(Im)_2$ using the bulky solvent system as structure-directing agents. ZIF phase transformations to denser phase from porous phase based on Ostwald rule of stages are discussed. Sophisticated control of solvent selection and reaction time showed the intriguing ZIF phase transformation (metastable to stable phase). The mentioned synthetic method suggests the importance of the intermediate phase during MOF crystal growth and modular synthesis toward desired porous materials.

Poster Presentation : **INOR.P-255**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Characterization of Electrospun nanofiber PCL/HAp and its biocompatible for Bone-marrow Mesenchymal stem cells

Nomundelger Gankhuyag, Ha Yun Jeong, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

Deformity in tissues can be healed by using a tissue engineering approach offering the development of biologically functionalized scaffolds from varieties of polymer and inorganic blends which mimic the extracellular matrix and allow adjusting the material properties to meet the defect architecture. Over the years, research interest has been shown towards the development of polycaprolactone (PCL) and Hydroxyapatite (HAP) based biomaterials for tissue engineering applications, because of its minimal foreign body reactions, biocompatibility, biodegradability, and ability to be molded into various geometries and forms thereby making it suitable for cell growth and differentiation. HAP can enhance alkaline phosphatase (ALP) activity in mesenchymal stem cells (MSCs), which is crucial as ALP activity plays a central role in the early mineralization process associated with bone formation. The present work involves the fabrication of nanofibrous scaffolds from PCL and HAP unified by the electrospinning method. The morphology and functional characteristics of the developed scaffolds were assessed by scanning electron microscopy and flow cytometric analysis. The scaffolds possess an adequate biodegradable, swelling, and mechanical property that is found desirable for tissue engineering applications. The cell study using a bone marrow-mesenchymal stem cell has confirmed the in vitro biocompatibility and cell differentiation supportive property of the scaffold thereby rendering their potentiality for future clinical applications.

Poster Presentation : **INOR.P-256**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Iron-catalyzed Borylation of Aryl Trifluoromethoxides

Jongheon Jeong, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Trifluoromethoxy group, which is a bioisostere of methoxy group and also fluorine-containing electrophile, has emerged as useful functional motifs in agrochemicals and pharmaceuticals due to their inherently high in vivo stability and lipophilicity. For this reason, introducing the trifluoromethoxy group to previously known fluorine or methoxy-containing bioactive molecules may be a useful methodology to adjust their metabolic stability, lipophilicity, or electron-withdrawing properties. Therefore, various methods for forging C(sp^2)–OCF_3 bonds have been studied. However, activation of C(sp^2)–OCF_3 bonds has garnered much less attention. There is no systematic study on the catalytic activation of C(sp^2)–OCF_3 bonds notwithstanding defluorinative functionalization has been extensively studied for new synthetic methodologies and environmental safety. Therefore, we paid attention to developing a method for the efficient functionalization of C(sp^2)–OCF_3 bonds. Herein, an iron-catalyzed detrifluoromethoxyborylation of aryl trifluoromethoxides is described. This reaction can be operated using a commercial iron salt and inexpensive ligand which can be easily synthesized in a single step without a complicated isolation process.

Poster Presentation : **INOR.P-257**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Coarsening-induced Hierarchically Interconnected Porous Carbon Polyhedrons for Stretchable Ionogel-based Supercapacitors

InCheol Heo, Won Cheol Yoo[1,*]

Department of Applied chemistry, Hanyang University, Korea
[1]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

Carbonaceous materials have received extensive attention as electrode materials for electrochemical energy storage systems owing to their superior features, including light weight, high electrical conductivity and specific surface area (SSA), tunable pore structures, and desirable surface properties. For ultrahigh-energy-density supercapacitors (SCs), hierarchically interconnected micro-/meso /macroporous carbons (HICs) are desirable for both effective ion polarization and transport, especially when electrochemically stable but dynamically sluggish ionic liquids are employed as the electrolytes. Herein, we demonstrate coarsening-induced HIC polyhedrons with an ultrahigh SSA (3064 m2 g−1) from polymer-infiltrated metal-organic frameworks (MOFs). The HIC-based SCs exhibit an outstanding capacitance of 268.4 F g−1 with an ultrahigh energy density of 149 Wh kg−1, which are comparable to the best values reported to date, indicating that expedited ion-transport via hierarchically interconnected large meso /macropores affords maximum utilization of the micropores of the carbon electrodes. Furthermore, stretchable all-solid-state SCs operating at 120% strain with a very high areal capacitance of 33 mF cm−2 and an energy density of 0.041 mWh cm−2 are also demonstrated. These results provide a ubiquitous strategy for developing MOF-based hierarchically interconnected carbonaceous materials with ultrahigh SSA for high-performance SCs compatible with stretchable and wearable electronic devices.

Poster Presentation : **INOR.P-258**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Observation of photoluminescence and single crystal X-ray diffraction : change of 1D ladder to 2D network.

Seok Kyun Jeong, Yu Jin Kim, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

$Zn(NO_3)_2$ with 2,4,6-tris(pyridine-3-yloxy)-1,3,5-triazine(L) were self assembled a 1D ladder metal complex and left in a 1,4-dioxane medium for one week transformed into a 2D networks metal complex. The structure of the two materials was confirmed through Single crystal XRD and difference in nature between the crystals was characterized by their PL spectra.

Poster Presentation : **INOR.P-259**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

The size effect of metal-organic framework driven copper oxide nanocatalysts on C_{2+} products selectivity in electrochemical CO_2 reduction

Sungjoo Kim, Hyunjoon Song*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

After since the carbon dioxide has revealed to be the major cause for modern environmental issues, a desire for producing C_{2+} products from electrochemical CO_2 reduction reaction (eCO_2RR) became one of the promising alternatives. Especially, copper-based nanocatalysts were regarded to be advantageous for producing C_{2+} products from eCO_2RR, since their moderate binding energy against CO* is able to promote dimerization. Recently, metal-organic framework (MOF) based/driven catalysts were gaining attention because of their facile synthesis and enhanced active sites. Herein, we prepared two copper-based MOFs with nanosized and microsized crystal, respectively and converted them into copper oxide form. The copper oxide catalyst prepared from nano-scaled MOF crystals exhibited improved selectivity toward C_{2+} products, compared to the catalyst fabricated from micrometer scaled MOF. The electrochemical performance of nano-scaled MOF driven copper oxide nanocatalysts was measured to be 81.2% of Faradaic efficiency toward C_{2+} products at −1.01 V versus reversible hydrogen electrode (vs. RHE).

Poster Presentation : **INOR.P-260**

Inorganic Chemistry

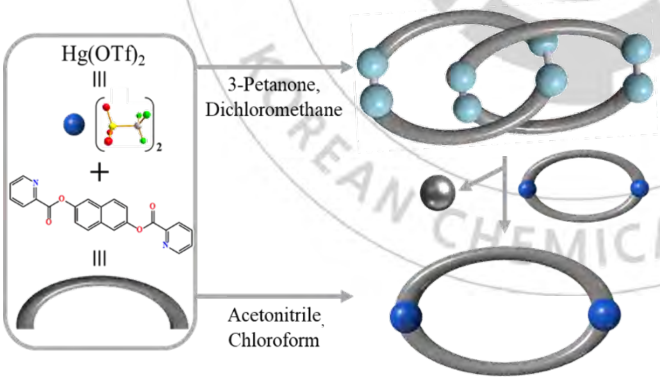
Event Hall FRI 11:00~13:00

Induced Transformation of Hg(II) complexes via Disproportionation

Dongwon Kim, Hyo Jeong Back, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

Self-assembly of of $Hg(OTf)_2$ with naphthalene-2,6-diyldipicolinate (L) in a mixture of 3-pentanone and dichloromethane produced the unusual catenated matallacycle of $[Hg_4(OTf)_4L_2]$ via straightforward formation of reduced Hg_2^{2+} as a skeletal synthon whereas the reaction in a mixture of acetonitrile and chloroform gave rise to metallacyles of $[Hg_2(OTf)_4L_2]$ via simple cyclization. The most important feature is that he successive addition of $[Hg_2\ (OTf)\ _4L_2]$ into $[Hg_4(OTf)_4L_2]$ in acetonitrile converged a product of $[Hg_2(OTf)_4L_2]$ quantitatively.



Poster Presentation : **INOR.P-261**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Identification of anisole adsorption ability by differences of metal and guest molecules

Gyeongwoo Kim, Gyeongmin Kim, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

New ligand tri(isoquinolin-5-yl) benzene-1,3,5-tricarboxylate are synthesized by isoquinolin-5-ol. Self - assembly of $Co(NO_3)_2$, $Ni(NO_3)_2$, $Cu(NO_3)_2$, $Zn(NO_3)_2$ with L as a tridentate N-donor. They are produced of 2D sheet structures. Despite being uniquely different group metals, they have the same crystal system, space group. In this 2D sheet, the solvent is present in the sheet and also between the sheet and the sheet. In the case of all metal complexes, it was observed that most solvents including decalin and xylene became guest exchanges. However, it was confirmed that the adamantane was not exchanged for the rest of the metal complexes except for the Co(II) complex. In this mode, the tetrahydrofuran solvate molecules were, in the present study, replaced for adsorption of 1,4-dioxane, anisole. In contrast, the 1,4-dioxane solvate molecules were replaced for adsorption of anisole. In this case, NMR monitoring about 1,4-dioxane and anisole was conducted. This crystal system, furthermore, could be useful as an efficient and tolerant crystalline matrix for molecular-structure determination of a wide range of cyclic hydrocarbons.

Poster Presentation : **INOR.P-262**

Inorganic Chemistry

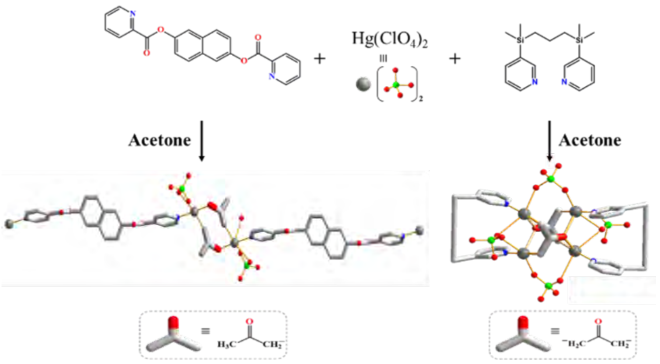
Event Hall FRI 11:00~13:00

Straightforward Formation of Monoanionic and Dianionic Acetonylate *via* Self-assembly of $Hg(ClO_4)_2$ with Ligands

Jihun Han, Hyeryeong Lee, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Acetone has known to exhibit the keto–enol tautomerism in which the nominal keto form $(CH_3)_2C=O$ of acetone itself is in equilibrium with its enol isomer $(CH_3)C(OH)=(CH_2)$. Thus, enolates derived from the deprotonation of carbonyl compounds are widely used as reagents in the synthesis of organic compounds. Enolate anions has known to be delocalized over the oxygen and the two carbon sites, and have the character of both an alkoxide and a carbanion. Deprotonation of such ketones gives enolates under vigrous condition such as strong bases, lithium diisopropylamide (LDA). Various metal–enolate species have been isolated by complexation with late-transition metal cations. According to Johnson's group, mercuration occurs spontaneously, if slowly, in acidic aqueous solutions of acetone and free mercuric ion to produce at least nine organomercury species including dianionic acetonylates, all of which can exist in equilibrium simultaneously. To the best of our knowledge, no examples of the X-ray structure on acetonyl coordination for mercury(II) complexes has been described at all. In this context, the present research will show the straightforward formation of the monoanionic and dianionic acetonylate species in both the solution and solid state.



Poster Presentation : **INOR.P-263**

Inorganic Chemistry

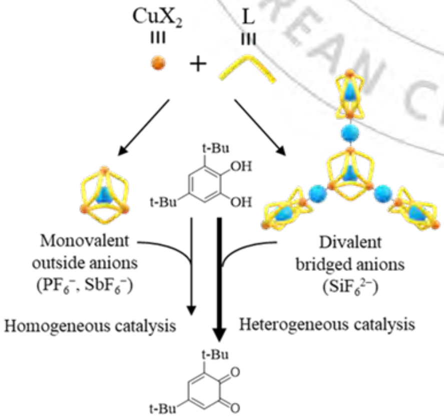
Event Hall FRI 11:00~13:00

Exceptional efficiency of heterogeneous catechol oxidation catalystin terms of structural properties

Geon Woo Gwak, Seonghyeon An, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of $Cu(BF_4)_2$ and $Cu(ClO_4)_2$ with ethyl(methyl)(3-pyridine)silane (L) as a bidentate N-donor. At the same time, $(NH_4)_2SiF_6$, NH_4PF_6, $NaSbF_6$ was added respectively. They produce new discrete cyclotrimeric rings and 4-fold interpenetrated coordination compounds. The coordination network acts as a remarkable catechol oxidation system that shows both of the significant counteranion effect and coordination skeleton effect. As the coordination compound has a smaller counteranion and reacts with less dissolution in the solution phase, compounds show the higher catalytic efficiency. Efficiency of the skeleton was confirmed by varying the degree of solubility of the compound, which is conducted by controlling reaction temperature and slightly changing the composition of the acetone solvent.



Poster Presentation : **INOR.P-264**

Inorganic Chemistry

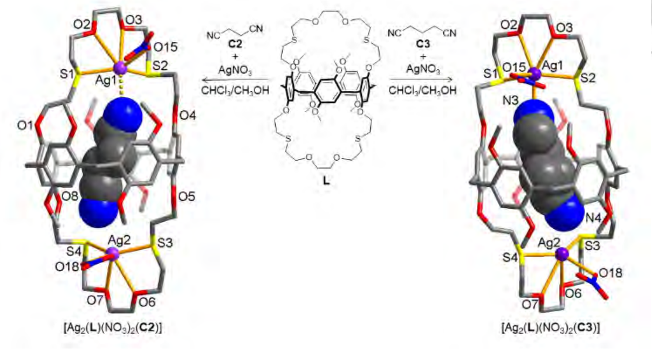
Event Hall FRI 11:00~13:00

Pillar[5]-*bis*-thiacrown as an Adaptive Tricyclic Host Exhibiting Selectively Recognizing Organic Guest via Dimetallation

Yelim Lee, Joon Rae Kim, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

In biomolecular recognition such as enzyme-substrate or protein-RNA, some host systems change their shapes in order to bind selectively to a suitable guest molecule. In this presentation, pillar[5]-*bis*-thiacrown (**L**) which contain flexible crown ether binding sites was synthesized to examine the guest molecule recognition on the coordination assembly with the metal ion. In the assembly reaction of **L** with α,ω-dicyanoalkanes [$CN(CH_2)_nCN$], n=2-6, (**C2–C6**), all organic guests exist in the pillararene cavities of **L** by supramolecular interaction. Reaction of **L** with organic guests in presence of silver(I) nitrate, meanwhile, silver(I) ions coordinated to the crown chains induced rigid conformational change for selective molecular recognition of organic guest. The longer guest than Ag…Ag distance of a disilver(I) complex was not recognized, indicating the proposed host is adapted via metallation for the length-selective recognition. The complexation studies of **L** with organic guests both in solution and solid states are in progress.



Poster Presentation : **INOR.P-265**

Inorganic Chemistry

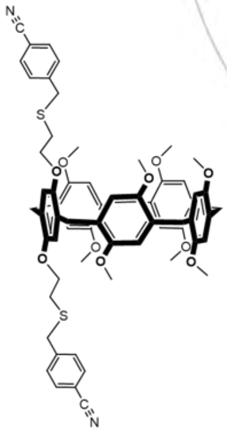
Event Hall FRI 11:00~13:00

Synthesis and Characterization of Pillar[5]arene Derivative having Benzonitrile Subunit and Their Metallosupramolecules

<u>Seo Hyeon Yun</u>, Yelim Lee, Joon Rae Kim, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

We proposed a pillararene derivative as a ditopic macrocycle which employs a pillar[5]arene moiety to accommodate one guest molecule in the cavity and the two benzonitrile subunits for the coordination networking. In this presentation, synthesis and structural characterization of the benzonitrile-containing pillar[5]arene (**L**) and its metallosupramolecules with soft metals are reported. **L** was synthesized from reaction between corresponding dibromide and 4-mercaptopyridine in the presence of K_2CO_3. The soft metal complexation behaviors of L and their structure-physical properties relationship are in progress.



L

Poster Presentation : **INOR.P-266**

Inorganic Chemistry

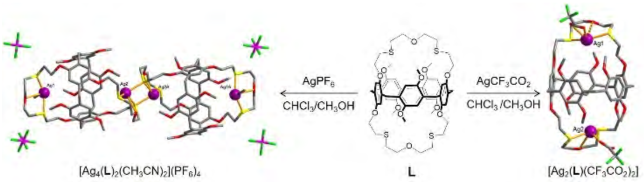
Event Hall FRI 11:00~13:00

Anion Effects on the Molecular Recognition and Coordination Networking of Silver(I) Complexes with Pillar[5]-bis-thiacrown

Joon Rae Kim, Yelim Lee, In-Hyeok Park[1], Eunji Lee[*]

Department of Chemistry, Gangneung-Wonju National University, Korea
[1]*Graduate School of Analytical Science and Technology, Chungnam National University, Korea*

One of challenging tasks in the supramolecular chemistry comes from how the coordinative networking might be influenced by controlling factor and how such phenomenon might be applied to selective organic recognition guests. Pillar[5]-*bis*-thiacrown (**L**) was employed to examine the guest molecule recognition on the coordination assembly with the metal ion.[1] The reactions of **L** with silver(I) salts (X = BF_4^-, $CF_3CO_2^-$, or PF_6^-) afforded the respective anion-dependent supramolecular complexes with different coordination modes. For examples, the reactions of **L** with $AgBF_4$ and $AgCF_3CO_2$ yielded isostructural disilver(I) complexes of type $[Ag_2\mathbf{L}(X)_2]_n$ (X= BF_4^- and $CF_3CO_2^-$). Meanwhile, the reaction of **L** with $AgPF_6$ afforded a bis(macrocycle) tetranuclear complex with the formula$[Ag_4(\mathbf{L})_2](PF_6)_4$.The organic molecular recognition of such silver(I) supramolecular complexes both in solid and solution states are discussed.Reference 1. E. Lee, H. Ryu, H. Ju, S. Kim, J.-E. Lee, J. H. Jung, S. Kuwahara, M. Ikeda, Y. Habata, S. S. Lee, *Chem. Eur. J.* **2019**, *25*, 949-953.



Poster Presentation : **INOR.P-267**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Effects of structural geometry around C-C bond axis on intramolecular charge transfer-based radiative decay in naphtyl- or quinoline- based *o*-carborane

Chan Hee Ryu, Kang Mun Lee[*]

Department of Chemistry, Kangwon National University, Korea

Naphthyl- and quinoline-appended *o*-carboranyl compounds, **NCB** and **QCB**, respectively, were prepared and fully characterized by multinuclear NMR spectroscopy, elemental analysis, and single crystal X-ray diffraction. Although both the compounds were non-emissive in the solution state at 298 K, they were photoluminescent in the rigid state (in THF at 77 K and film state) in the region 450–550 nm. Theoretical calculation of the optimized structure in the S$_1$ state suggested that the low-energy emissive bands for **NCB** and **QCB** were attributed to intramolecular charge transfer (ICT) transition. Intriguingly, the C−C bond axis of the *o*-carborane in **NCB** in the solid state was more orthogonal to the plane of the appended aromatic group than that in **QCB**, indicating relatively high delocalization between the *o*-carborane and aromatic moieties of **NCB**. The quantum efficiency and radiative decay constant of the ICT-based emission of **NCB** in the film state were much higher than those of **QCB**. These findings suggest that the structural geometry around the C−C bond axis of the *o*-carborane is a crucial factor in accelerating the ICT-based radiative decay in the *o*-carbonyl luminophores in the rigid state.

Poster Presentation : **INOR.P-268**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Strategic molecular design of *o*-carboranyl 1*H*-phenanthro[9,10-*d*]imidazoles to enhance efficiency of intramolecular charge transfer-based luminescence

Sanghee Yi, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Herein, we prepared and characterised a series of 1*H*-phenanthro[9,10-*d*]imidazole-based *o*-carboranyl compounds (**_o_PC**, **_m_PC**, **_p_PC**, and **PC**) and compared their optical properties. **_o_PC** and **_m_PC** exhibited only high-energy emissions attributed to locally excited transition centred at ~380 nm in solution at 298 K and a dual-emissive pattern in high-energy ($\lambda_{em} \approx 385$ nm) and low-energy ($\lambda_{em} \approx 580$ nm) regions due to a LE and intramolecular charge transfer (ICT)-based emission in the rigid state (THF solution at 77 K and film), respectively, while **_p_PC** and **PC** exhibited ICT-based emission only in the rigid state. Compared to **_o_PC** and **_m_PC**, **_p_PC** and **PC** demonstrated considerably higher Φ_{em} and k_r values for ICT-based emission in the film state. Analysis of solid-state structures revealed that the C–C bond axis of the *o*-carborane was orthogonal to the plane of the appended aromatic group for **_p_PC** and **PC** but not for **_o_PC** and **_m_PC**. Theoretical calculations of the low-energy transition in the first excited states of **_p_PC** and **PC** upon the rotation of the *o*-carborane cage verified that the above orthogonality plays an important role in the maximisation of ICT-based luminescence. These results demonstrate that the structural geometry around the *o*-carborane cage is a critical factor for controlling the ICT-based radiative decay of *o*-carboranyl luminophores.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-269**

Inorganic Chemistry

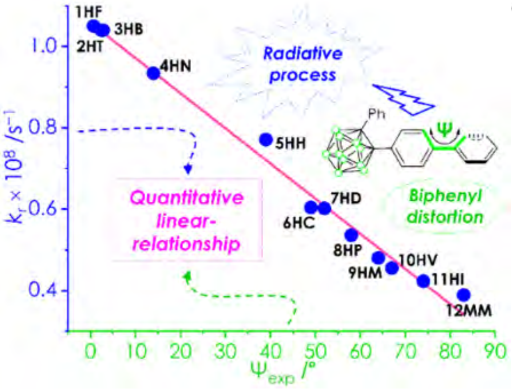
Event Hall FRI 11:00~13:00

Quantitative relationship between structural distortion and intramolecular charge transfer-based radiative process in biphenyl-based *ortho*-carborane

Mingi Kim, **Kang Mun Lee**[*]

Department of Chemistry, Kangwon National University, Korea

Herein, 13 *o*-carboranyl compounds that contain specific geometries, ranging from planar to orthogonally distorted biphenyl rings, were synthesized and structurally characterized to establish the effect of structural formation of the aromatic group attached with the *o*-carborane to efficiency for their radiative decay process. All the compounds showed significant intramolecular charge transfer (ICT)-based emission in the crystalline state at 298 K. Interestingly, increasing the distorted dihedral angles between biphenyl rings gradually decreased the emission efficiencies. Moreover, their radiative decay constants decreased linearly with increasing dihedral angle, which demonstrated the inversely proportional relationship between these two factors. The results of this study distinctly suggest that the planar or distorted geometry of substituted aryl groups can strongly affect the efficiency of the ICT-based radiative process in *o*-carboranyl luminophores.



129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **INOR.P-270**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Proton conductivity on MOF using sulfonate groups

Seungjae Park, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Metal-organic frameworks (MOFs) are representative robust and porous crystalline materials consisting of metals and organic linkers. In the past few decades, numerous metal-organic frameworks (MOFs) and their synthetic methods have been reported to develop their interesting applications tuning their clusters and linkers. Typically, the gas separation[1,2], catalysis[3], and conductivity[4] are investigated for their applications. In this study, proton conductive material was synthesized with rigid structure and high conductivity. The material was synthesized by zinc and monosodium 2-sulfoterephthalate as the linker. Three different structures were obtained in different synthetic conditions. It was characterized by the powder X-ray diffraction, gas adsorption, and conductivity on various temperature and relative humidity.

Poster Presentation : **INOR.P-271**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

The Photo-Switchable Behavior Controlled by Intermolecular Interaction of Azobenzene-Containing Polyamide Films Growth by Molecular Layer Deposition

Sung ho Kim, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

Photo-sensitive polymer film has been attracted in the field of material science including biological system and optical devices which are sensitive on the change of surface topology. Recently, azo compound (R-N=N-R'), as one of the photo-induced reversible transformation unit, has been highlighted in the research related photo-sensitive polymer film including surface science, artificial muscle, biological and optical application, because light used as external triggers for inducing surface transformation is manageable to control without modification of nano-structures and environment concerns.In this study, we fabricated photo-reversible polyamide film based on coupling reactions between azobenzene-4, 4'-dicarbonyl dichloride (Azo) and hexamethylenediamine (HDA) by molecular layer deposition through self-limiting surface reaction. And, we investigated the photo-induced reversible transformation of azobenzene-containing polyamide thin film. In situ Fourier Transform Infrared (FTIR) measurement was used to monitor the growth of polyamide film, and the light-induced transformation was characterized by UV-vis spectroscopy. In addition, to measure the surface potential energy in azobenzene-containing polyamide film, scanning kelvin probe microscopy (SKPM) was used.

Poster Presentation : **INOR.P-272**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Regulating the Phenotypic Polarization and Adhesion of Macrophage by Topographical Cue

Yoobeen Lee, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

Successful wound healing and complete tissue integration using biomedical materials are mainly determined by inflammatory reactions. Macrophages play a central role in determining the degree of inflammatory response and their activity in response to the scar and implant surface is known to affect the subsequent healing outcome. Nanoscale topographical modification in the design of the surface is important process for enhancing healing capacity. Here, we fabricate close packed hexagonal array with different diameter of silica nanobeads affect on focal adhesion establishment and maturation. Our data showed that macrophages seeded on small sized nanobead surfaces tended to induce macrophages toward a pro-inflammatory (M1) phenotype with more pro-inflammatory cytokine secretion and marker expression. On the other hand the macrophages seeded on large sized nanobead surfaces tended to induce macrophage toward an anti-inflammatory (M2) phenotype with more anti-inflammatory cytokine secretion and marker expression compared to those on surfaces with a small sized bead surfaces. Our studies demonstrate that alterations in cell adhesion associated with changes in ECM structure may provide topographical cues to regulate macrophage phenotypic polarization.

Poster Presentation : **INOR.P-273**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Cellular Behavior Control of NIH/3T3 Fibroblasts on the Nano-topography with Curvature controlled using Liquid Phase Deposition

Yeon-su Yu, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

Biochemical cues ignore cellular microenvironments such as cell to cell interaction and extracellular matrix (ECM). Since the cells in vivo are communicated with ECM and cell-to-cell interaction, studies of topological cues are associated with cell in vivo. In recent year, various studies have shown that nano-topological cues regulate cell behavior such as cell adhesion, cell proliferation, migration, polarity, and differentiation. Although many previous studies have investigated cell behavior using various topographical cues, the results have meant topographical confinement by nanostructured architecture. Therefore, it is essential for surface topography to be studied through controlling the size, shape and density of the nanostructure. In previous study, we investigated the effects of the hexagonally close-packed silica bead arrays on cellular behavior, especially adhesion and proliferation. In this study, the size of the beads was kept constant and the curvature of the beads was adjusted by Liquid phase deposition (LPD) to control the degree to which cells adsorbed to the surface, and accordingly, the behavior of the cells was examined. LPD is a useful method for the deposition of oxide films at low temperatures under aqueous conditions. Using this process, the oxide films were produced without the use of electrochemical methods, vacuum systems, or sensitive organometallic precursors. As the LPD reaction time increases, the surface becomes flatter, and accordingly, the adsorption, migration, and speed of cells change as cells adsorb onto the nano-topography change.

Poster Presentation : **INOR.P-274**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and structural analysis of one-dimensional zinc coordination polymer with tetrazolyl ligand

Ga Hee Noh, Junseong Lee*

Department of Chemistry, Chonnam National University, Korea

Tris(pyrazolyl)borates complex, called as ‘scorpionate’, is a tridentate ligand system and considered as a quite useful tridentate ligand. It occupied one facial site and acted quite similarly with cyclopentadienyl ligand, providing broad applications in the field of supramolecular assembly, catalysis, and enzyme modeling. Despite the design similarities, strongly donating scorpionates differ in their topology and flexibility, donor properties and degradation pathways. The structural and electronic properties of these ligands are contrasted and related to their chemistry, particularly that of the transition metals. Recently, we already reported report formation of a new metallascorpionate ligand, [FeL3] 3− (IPtz), containing a Fe core and three 5- (2-hydroxyphenyl)-1H-tetrazole (LH2) ligands. It features two different binding sites, oxygen and nitrogen triangles, which consist of three oxygen or nitrogen donors from tetrazole. The binding affinities of the complex for three alkali metal ions were studied using UV spectrophotometry titrations.A K–FeTz3–K trimetallic complex was constructed by assembly of a tetrazolyl ligand, K, and Zn precursors and characterized using X-ray crystallography. Interestingly, high dimensional zinc coordination polymer was achieved and its structure was also confirmed by X-ray crystallography. In the structure, unprecedented one-dimensional zinc ions array was observed. In this presentation, the detailed synthesis and characterization of the 1-D zinc coordination polymer is discussed. The ability of strongly donating scorpionate ligands to stabilize metal ligand multiple bonds in late transition metal complexes is also briefly discussed.

Poster Presentation : **INOR.P-275**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

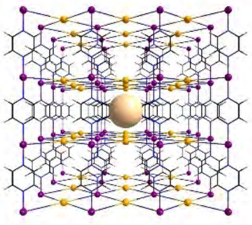
Hydrogen Isotope Separation in Hofmann-type Metal-Organic Frameworks with High-Density Open Metal Sites

Junsu Ha, **Hyunchul Oh[1,*]**, **Hoi Ri Moon[*]**

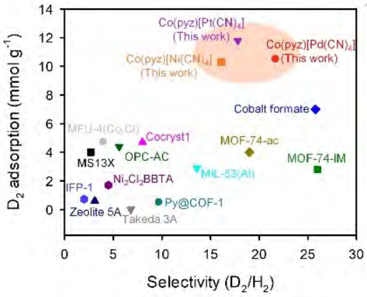
Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

[1]*Department of Energy Engineering, Gyeongsang National University, Korea*

Deuterium (D_2) possesses a critical role in various scientific areas such as biomedical applications, nuclear fusion and energy resource. Despite the high demand, D_2 separation from hydrogen isotopes is very challenging because of its identical physicochemical properties among the isotopes and extremely low natural abundance (0.0156 %). Conventional D_2 production methods such as cryogenic distillation and Girdler sulfide process only provide low separation factor (~ 2.5) at low temperature (20–25 K) with large energy consumption. Herein, we prepared Hofmann-type MOFs, $Co(pyz)[M(CN)_4]$ (M = Pd, Pt, and Ni) having high-density open metal sites (OMSs) for highly efficient isotope separation based on chemical affinity quantum sieving (CAQS). These MOFs show high separation factor ($S_{D2/H2}$) of 16.1–21.7 as well as high D_2 uptake of 9.7 – 11.2 mmol/g at 25 K. These are attributed to the high density of OMSs in the Hofmann-type MOFs.



Hofmman-type MOF



Poster Presentation : **INOR.P-276**

Inorganic Chemistry

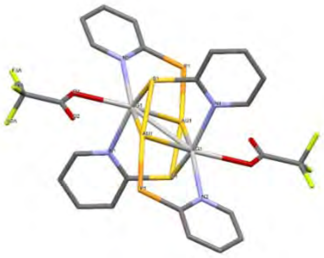
Event Hall FRI 11:00~13:00

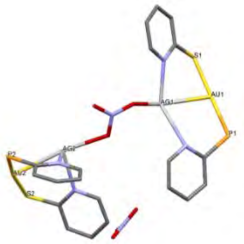
Anion effects of Au(I)···Au(I) *vs* Au(I)···Ag(I) interactions in d^{10} metal complexes

Jiyeong Song, Young-A Lee*

Department of Chemistry, Jeonbuk National University, Korea

The heterometallic Au(I)-Ag(I) complexes, [AuAg(Spy)(PPh$_2$py)]X (X = BF_4^-, PF_6^-, SbF_6^-, NO_3^-, ClO_4^-, $CF_3CO_2^-$, $CF_3SO_3^-$), have been synthesized and their physical properties were studied. According to the change of anion, it showed control of metal-metal interaction with the competition of d^{10} metals. X-ray characterizations on the single crystals have provided the dimeric (X = $CF_3CO_2^-$, $CF_3SO_3^-$, SbF_6^-) or polymeric form (X = NO_3^-, BF_4^-) of [AuAg(Spy)(PPh$_2$py)]X depending on the anion types. For the complexes with X = $CF_3CO_2^-$, the [AuAg(Spy)(PPh$_2$py)] moiety are bound via the transannular Au···Au interaction (5.050Å), Ag···Ag interaction (3.069Å) and bridging sulfur (Ag(1)···S(1): 2.54Å, Au(1)′···S(1): 2.33Å). Despite the similar skeletal structure, complexes with X = NO_3^-, show the infinite chains through the additional Au···Au interactions (2.98Å) and anion binding effects. These materials are luminescent in the solid-state and exhibit an emission band at 470nm (λ_{ex} = 360nm) at 77K and 560 nm peaks are slight.





Poster Presentation : **INOR.P-277**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Hydrogen Isotope separation by Zeolitic lmidazolate Franeworks(ZIF-67)

Hyunchul Oh*, Seulji Lee[1]

Department of Energy Engineering, Gyeongsang National University, Korea
[1]*Energy Engineering, Gyeongsang National University, Korea*

High-purity deuterium is used as a core fuel of nuclear fusion power generation and can be exploited in various industries and research as a future high-tech element, increasing its demand steadily. However, its separation of isotope mixture is quite challenging due to the almost identical size, shape and thermodynamic properties, making it difficult to apply a general gas mixture separation technique. Recently, to economically and efficiently separate hydrogen isotopes, kinetic quantum sieving (KQS) in crystalline nanoporous materials has drawn attention. Hence, in this study, hydrogen isotope adsorption behavior was studied using a chemically stable Zeolitic lmidazolate Franeworks(ZIF), capable of designing various shapes and pore sizes using metal ions such as Zn and Co. In particular, ZIF-67 possesses a small aperture size appropriate for hydrogen isotope separation, resulting in an efficient kinetic quantum sieving.

Poster Presentation : **INOR.P-278**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Electrochemical catalytic activity of S-doped Pd nanocubes for ethanol oxidation depending on morphological change controlled by the degree of sulfurization

Jae Eun Choi, Sambath Baskaran[1], Jaehoon Jung[2,*], Jong Wook Hong[*]

Chemistry, University of Ulsan, Korea
[1]*Chemistry, University of Ulsan, India*
[2]*Department of Chemistry, University of Ulsan, Korea*

Nanoparticle-based catalysts have been intensively studied not only due to their controllability via size, shape, and composition but also due to economic efficiency with high surface-to-mass ratio. Doping of nanoparticle with non-metallic elements has received an increasing attention as a way to improve the electrochemical performance by inducing high electron population at the surface of nanoparticle. We herein present the electrochemical investigation for sulfur-doped Pd nanocube as a electrochemical catalyst for ethanol oxidation which produces carboxylate species. The morphology of S-doped Pd nanocube depending on the degree of sulfurization, which is closely related with its electrochemical catalytic activity, was systematically examined with SEM, TEM, HAADF-STEM, and EDS measurements. The S-doped Pd nanocube became amorphous from the edge of nanocube as the concentration of sulfur increases. Furthermore, the optical concentration of sulfur leading to the highest catalytic activity was found to be 3 mM indicates a strong correlation between the electrochemical catalytic activity of S-doped Pd nanocube and its morphological change. The density functional theory calculations were also performed to elucidate the relation between surface composition and electrochemical catalytic activity. Our study suggests that the catalytic activity of nanoparticle can be finely controlled by doping non-metallic species.

Poster Presentation : **INOR.P-279**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Hydrogen isotope separation by using Metal organic frameworks (MOF-303)

Hyunlim Kim, Jaewoo Park[1], Hyunchul Oh[1,*]

Ulsan National Institute of Science and Technology, Korea

[1]*Chemistry, Ulsan National Institute of Science and Technology, Korea*

Recently, Demand for Deuterium (D_2) has risen manifold due to its usage for many scientific applications, including its usage as a fuel for the nuclear fusion process. However, the very low natural abundance, its separation requires more serious efforts. The conventional gas separation method based on the size exclusion principle is not helpful due to similar physicochemical properties of H_2 and D_2. Moreover, the existing D_2 separation methods like cryogenic distillation, Girdler sulfide (GS) method, and thermal diffusion and centrifugation are not energy efficient. Adsorption-based separation using high surface area material has shown promising results. Among them, MOFs are employed exclusively because of their high specific surface area, controllable pore size, and well-defined physiochemical properties. So herein, we explore MOF-303 having high specific surface area (SSA) of 1240 m^2/g. The isotope separation properties were analyzed using advanced cryogenic thermal desorption spectroscopy (ACTDS). ACTDS measurements showed that D_2/H_2 selectivity ($S_{D2/H2}$) at 25 K was higher compared to $S_{D2/H2}$ at 40 K, and it could be ascribed to enhanced kinetic quantum sieving effect at low temperature. Interestingly, $S_{D2/H2}$ increased with increasing loading pressure, with a maximum $S_{D2/H2}$ of 21 at 1 bar and 25 K. These observations indicate that MOF-303 can efficiently separate H_2 isotopes.

Poster Presentation : **INOR.P-280**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Exploiting Dynamic Opening of Cavity in Fluorinated Porous Polymers for Enhancing Hydrogen desorption temperature and isotope separation

Minji Jung, Hyunchul Oh*

Chemistry, Ulsan National Institute of Science and Technology, Korea

Nuclear fusion has been considered a promising and clean energy source and can solve the anticipated energy crisis. Deuterium (D_2) is fuel for the nuclear fusion process, making it crucial considering the demand for clean energy in the future. However, its natural abundance is quite low, and its separation from the hydrogen isotope mixture is also challenging due to its identical size, shape, and thermodynamic properties. Currently, D_2 can be separated either by using the Girdler sulfide process(GS) or Cryogenic distillation, but these two methods entail low separation efficiencies and high energy consumption. Hence, it necessitates the development of more efficient separation technology. Recently, D_2 separation from hydrogen isotope mixture using crystalline nanoporous materials through quantum sieving effect has been launched as a promising and cost-effective approach. Herein, we report the investigation of hydrogen isotopes separation using cost-effective, flexible fluorinated porous polymer through home-built cryogenic thermal desorption spectroscopy (TDS) equipped with quadrupole mass spectroscopy (QMS). TDS measurement was performed by directly introducing the D_2 and H_2 mixture with 1:1 composition to the sample and D_2/H_2 selectivity was obtained after careful calibration by PdCe alloy and TiH_2. The selectivity was affected by the experimental conditions such as temperature, gas pressure, and exposure time, which could be ascribed to the experimental conditions driven transition of the flexible structure of the framework. Moreover, the experimental conditions for the efficient separation of hydrogen through flexible fluorinated porous polymer have been optimized to improve separation performance. The obtained results indicate that flexible fluorinated porous polymers can be used as an alternative material for hydrogen isotopes separation.

Poster Presentation : **INOR.P-281**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Structural and anion effects of Zinc(II) Coordination Polymers on 4-Nitrophenol Sensing Properties

Hyemin Lee, Haeri Lee*

Department of Chemistry, Hannam University, Korea

In nature, bio-active supramolecules such as enzymes and antibodies can activate guest molecules, which plays a key role in the introduction of molecular functions to achieve designated functions. In this research, to synthesize transition metal complexes and to examine a sensing effect depending on the structures and solubility, nitrogen donor ligand was designed and synthesized. Zinc(II) coordination polymers were synthesized and characterized by single crystal X-ray diffraction and used for sensing 4-nitrophenol.

Poster Presentation : **INOR.P-282**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Self-assembly and Spectroscopic Analysis for Zinc(II) Coordination Polymers

Inhye Kim, Haeri Lee*

Department of Chemistry, Hannam University, Korea

Metal complexes have higher crystallinity and thus better physical properties by better controlling the three-dimensional regularity of polymers to generate syntactic or isotopes. And there is an advantage of being able to form a polymer having a higher molecular weight. Metal-organic materials has been known as many applications such as catalysts, dyes, molecular storages. Construction of metal organic structures is strongly dependent on the design of ligands and choice of metal precursors. In my research, coordination polymers consisting of zinc(II) and imidazole donor ligand were synthesized. Zinc(II) has six coordinations and forms an octahedron, so it shows a stable and regular arrangement when synthesized with a ligand to form a zinc complex. In order to obtain zinc(II) complexes, we designed bidentate N-donor ligand containing imidazole group. After synthesis, ligand introduced that the physicochemical properties of the complex were investigated through single crystal X-ray structure analysis and spectroscopic analysis. Reaction of L and zinc(II) metal precursor produced 1D coordination polymers. According to anions and solvent system, 1D polymers packed in a different way.

Poster Presentation : **INOR.P-283**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Construction and Structural Analysis of Copper(II) 2D Network Structures

Eunbi Jeong, Haeri Lee*

Department of Chemistry, Hannam University, Korea

To obtain copper(II) compounds, self-assembly method was used. The copper(II) compounds can be obtained by experimenting copper(II) and N-donor ligand in H2O/acetone, H2O/EtOH and EtOH/CHCl3 mixture. The structure of copper compounds represents that a copper(II) metal center coordinates four ligands and two anions.

Poster Presentation : **INOR.P-284**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Highly efficient blue electroluminescence devices based on Au(I) complexes as ultrafast triplet exciton harvesters

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Thermally activated delayed fluorescence (TADF) molecules have emerged as the promising alternatives to phosphorescent emitters in high-efficiency organic light-emitting devices (OLEDs). However, OLEDs based on blue TADF emitters developed thus far hardly meet the rigorous conditions for commercialization with respect to the efficiency, color purity, and stability. In particular, hyperfluorescence OLEDs employing TADF emitters suffer from severe roll-off in efficiencies due to bimolecular exciton annihilation which is attributed to slow reverse intersystem crossing (rISC) rates from organic exciton sensitizers. In this research, we have developed hyperfluorescence electroluminescence devices employing Au(I) complexes as singlet exciton sensitizers. The complexes consist of an N-heterocyclocarbenic ligand with 1,3-bis(2,6-diisopropylphenyl)-1H-benzo[d]imidazol-2-ylidene (^{Dipp}BZI), and 1,3,6,8-tetramethyl-9H-carbazolide (TMCz) or carbazolide (Cz) ligands. Our Au(I) complexes are capable of ultrafast singlet exciton harvest attributed to rapid rISC rates at $\sim 10^{8}$ s-1. OLEDs involving multi-resonance TADF molecules as the emitting dopants, together with the Au(I) complex exciton sensitizers, produced an external quantum efficiency as high as 30.2% and a narrow full width at half-maxium of 20 nm in the blue region. The devices also exhibited a reduced roll-off in efficiencies and longer operational lifetime by one order of magnitude compared to control devices based on organic exciton sensitizers.

Poster Presentation : **INOR.P-285**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Single metal–organic framework (MOF)-embedded nanopit arrays: A new way to control neural stem cell differentiation.

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Stable and continuous supply of essential biomolecules is critical to mimic in vivo microenvironments wherein spontaneous generation of various cell types occurs. Here, we report a new platform that enables highly efficient neuronal cell generation of neural stem cells using single metal–organic framework nanoparticle (MOF)-embedded nanopit arrays (SMENA). By optimising the physical parameters of homogeneous periodic nanopatterns, each nanopit can confine single nMOFs (UiO-67) that are specifically designed for long-term storage and release of retinoic acid (RA). The SMENA platform successfully inhibited physical interaction with cells, which contributed to remarkable stability of the nMOF (RA$\subset$UiO-67) structure without inducing nanoparticle-mediated toxicity issues. Owing to the continuous and long-term supply of RA, the neural stem cells showed enhanced mRNA expressions of various neurogenesis-related activities. The developed SMENA platform can be applied to other stem cell sources and differentiation lineages and is therefore useful for various stem cell-based regenerative therapies.

Poster Presentation : **INOR.P-286**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Effect of ancillary ligand on the photoluminescent properties of blue Ir(III) complexes bearing main bipyridine ligand through computational study

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During the past two decades, there has been considerable interest in the design of phosphorescent transition metal Ir(III) and Pt(II) complexes based on C^N chelates. These materials exhibit strong emissions from blue to yellow depending on either ligand frameworks or the presence of strong intermolecular interactions. Due to the importance of Ir(III) complexes for blue OLEDs, it is of great interest to investigate 2,3′-bipyridine classes of Ir (III) complexes in more detail. We have focused on dfpypy because bipyridine-based Ir(III) compounds have exhibited significantly blue-shifted emissions, which is attributed to the electronegative pyridine ring compared to other irdium compounds with chelating C^N ligands. To elucidate the origin of the photophysical properties for homoleptic and heteroleptic cyclometalated blue Ir(III) complexes by density functional theory (DFT) calculations and understand the difference of photoluminescent quantum efficiencies (PLQYs) and aggregation between two iridium(III) complexes, the permanent dipoles were also investigated. As a result, an ancillary ligand was more effective in elevating the HOMO as well as LUMO energy levels without considerably altering the energy gap with respect to its homoleptic counterpart, thus significantly influencing the performance of the Ir(III) compounds in phosphorescent organic light-emitting diodes (PhOLEDs). Also the electronic transition for homoleptic Ir(III) compound may be attributed to the combination of ILCT, ($\pi_{bpy}-\pi^*_{bpy}$), and MLCT, ($Ir_d-\pi^*_{bpy}$), while for heteroleptic Ir(III), it may be because of the combination of ILCT and MLCT along with LLCT, ($\pi_{acac}-\pi^*_{bpy}$).

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Poster Presentation : **INOR.P-287**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Structure and Electrophilic Reactivity of Non-Porphyrinic Manganese(IV)–Hydroxide Complexes

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We report the single crystal X-ray structure and spectroscopic characters of a mononuclear non-porphyrinic Mn^{IV}–(OH) complex, $[Mn^{IV}(Me_3\text{-TPADP})(OH)(OCH_2CH_3)]^{2+}$ (**2**), using various physicochemical methods. Likewise, $[Mn^{IV}(Me_3\text{-TPADP})(OH)(OCH_2CF_3)]^{2+}$ (**3**) which is thermally stable at room temperature was also synthesized and characterized spectroscopically. Further, the Mn^{IV}–(OH) adducts perform oxidation reactions with external organic substrates. Hammett correlation, kinetic isotope effect and product analyses demonstrate that **2** and **3** exhibit electrophilic oxidative reactivity toward hydrocarbons. DFT calculations support the assigned electronic structure and show the direct C–H bond activation of the Mn^{IV}–(OH) species is possible.

Poster Presentation : **INOR.P-288**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Structural Design of Novel Anti-Reflective Nanostructure by integrating a MgF_2 Single Light-Interference Layer with a SiO_2 Moth-Eye Nanostructure

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The importance of light reflection loss, referred to as the Fresnel loss, has been increasing in certain opto-electronic devices since the Newtonian era. Generally, a simple but difficult method to decrease light reflection involves adjusting a single impedance-matched layer such as a MgF_2 layer on a glass substrate. Another commonly known anti-reflective (AR)-coating method is to decrease the refractive index gradually, approximating the moth-eye nanostructure in nature. In this study, we attempt to combine the advantages of each AR-coating method, analyzing the parameters that are mainly linked to a reduction in the Fresnel loss. Here, we introduce a newly developed broadband AR nanostructure on the front side of a glass/indium tin oxide (ITO)/perovskite solar cell (PSC) by integrating a single layer interference effect with a moth-eye like nanostructure to reduce the Fresnel loss. Moreover, we demonstrate a relationship between the structural parameters of the nanopatterned AR nanostructure. The best optimized condition of the newly developed AR nanostructure was simulated by a finite-difference time-domain (FDTD) analysis. To ensure the veracity of the simulated results, we controlled various dimensions of the SiO_2 moth-eye nanostructure and the thickness of the MgF_2 single layer, after which the best optimized condition, which had a 100 nm MgF_2 film coated onto the SiO_2 moth-eye nanostructure (165 nm diameter and 400 nm height), was demonstrated. As a result, the high-efficient newly developed AR coated PSC with power conversion efficiency of 20.48% (PCE) was introduced, showing an increased short-circuit current density of 11.80% (J_{SC}) and PCE of 12.50%.

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Poster Presentation : **INOR.P-289**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Development of *Operando* EPR for Electrochemical Catalysts

Sugyeong Hong, Sun Hee Kim[*]

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Electron Paramagnetic Resonance (EPR) spectroscopy is a powerful spectroscopic method for analyzing the structure, reactivity in paramagnetic complex with unpaired electrons. In addition, it is possible to analyze the structure of intermediate species and the surrounding environment during chemical reactions. However, if the life-time of the intermediated species produced by the electrochemical reaction is very short, the EPR spectroscopy may be difficult to be applied. Due to the short life-time of intermediate species during electrochemical reaction, it is difficult to capture intermediates, thus the catalytic reaction is hard to be clarified. The *operando* EPR system is a means to complement the limit of the *ex-situ* EPR spectroscopy. The *operando* EPR system is a technique for measuring EPR spectroscopy at the same time as another reaction in progress. This approach makes it easier to overcome the limitations of the *ex-situ* EPR spectroscopy, and furthermore to track changes in the product over the electrochemical reaction time. When an *operando* EPR experiment is being conducted including aqueous solutions, a common EPR cell can not be used. A new EPR cell which has significantly reduced the volume of the part corresponding to the EPR spectroscopy measurement area is in use. In this presentation, we present a new EPR cell to find an essential clue to comprehend the electrochemical reaction mechanism.

Poster Presentation : **INOR.P-290**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Transient EPR spectroscopic investigation of the excited triplet states of anthracenes

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Transient EPR(TR-EPR) is an EPR technique to probe excited state triplets of molecular systems as a nanosecond time resolution. Once the light is irradiated, triplet state would be generated by the excitation of light, and EPR measurements would be conducted during light irradiation. TR-EPR can be used to monitor the spin state, spin population, and characterization of excited species. Moreover, it can also provide pivotal evidence to a variety of important mechanisms that are mediated by the triplet species.In this presentation the representative experimental results of TR-EPR will be presented. In the first part, the TR-EPR results of the iridium complexes will be reported with electron acceptor molecules by irradiation of 355 nm pulse laser. In the second part, the TR-EPR results of anthracene derivatives will be presented with comparing different functional groups of anthracene derivatives. In addition, we probed the electronic structure of the triplet state of anthracene derivatives with ENDOR spectroscopy. These results provide TR-EPR can be a powerful tool to understand the properties of excited triplet states.

Poster Presentation : **INOR.P-291**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Nominally stoichiometric $Na_3(W_xSi_xSb_{1-2x})S_4$ as a superionic solid electrolyte

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Na_3MX_4 (M = P, Sb and X = S, Se) and its doped analogues are considered as a promising material in realizing room-temperature (RT) Na^+ -conducting solid electrolytes. Herein, we first report that stoichiometric $Na_3(W_xSi_xSb_{1-2x})S_4$ with no nominal vacancies shows significantly high ionic conductivity at RT (σ^{RT}) when compared with Na_3SbS_4. The σ^{RT} is continuously increased with increasing ‘x’, and the highest σ^{RT} and the lowest activation of 13.2 mS·cm^{-1} and 0.16 eV, respectively, are reached in cubic $Na_3(W_{0.2}Si_{0.2}Sb_{0.6})S_4$. Further increase of ‘x’ results in the formation of a glassy phase and a decrease of σ^{RT}. Such a high σ^{RT} of $Na_3(W_{0.2}Si_{0.2}Sb_{0.6})S_4$ suggests that another factor such as a dynamic motion of MS_4 tetrahedra can affect Na^+ diffusion in addition to structural defects. Ab-initio molecular dynamics also reveal that the improvement of σ^{RT} with increasing ‘x’, but the presence of naturally formed vacancies, which is the common phenomenon in Na_3MX_4. The electronic conductivity of $Na_3(W_{0.2}Si_{0.2}Sb_{0.6})S_4$ is also low (ca. 10-6 mS·cm^{-1}). Unfortunately, cathodic stability becomes worse with W^{6+}/Si^{4+} co-doping due to mismatch in soft-acid/soft-base chemistry. Therefore, a full cell ($Na_{15}Sn_4 \| TiS_2$) is fabricated with an interlayer of Na_3SbS_4 between $Na_{15}Sn_4$ and $Na_3(W_{0.2}Si_{0.2}Sb_{0.6})S_4$, and its performance is demonstrated.

Poster Presentation : **INOR.P-292**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Acridine based small molecular hole transport type materials for phosphorescent OLED application

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Two small molecular hole transporting type materials, namely 4-(9,9-dimethylacridin-10(9H)-yl)-N-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)-N-phenylaniline (TPA-2ACR) and 10,10'-(9-phenyl-9H-carbazole-3,6-diyl)bis(9,9-dimethyl-9,10-dihydroacridine) (PhCAR-2ACR) were designed and synthesized using a single step Buchwald-Hartwig amination between the dimethyl acridine and triphenylamine or carbazole moieties. Both materials showed high thermal decomposition temperatures of 402 and 422 oC at 5% weight reduction for PhCAR-2ACR and TPA-2ACR, respectively. TPA-2ACR as hole transporting material exhibited excellent current, power, and external quantum efficiencies of 55.74 cd/A, 29.28 lm/W and 21.59%, respectively. The achieved device efficiencies are much better than that of reference 1,1-Bis[(di-4-tolylamino)phenyl]cyclohexane (TAPC) based similar device (32.53 cd/A, 18.58 lm/W and 10.6%). Moreover, phenyl carbazole based PhCAR-2ACR showed good device characteristics when applied for host material in phosphorescent OLEDs.Keywords: Organic light emitting diodes; HTL; Host material; Acridine; Triphenylamine; Carbazole.

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Poster Presentation : **INOR.P-293**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Impact of Surface Termination of Sapphire Substrate on Crystallographic Epitaxial Growth of Highly-Oriented Monolayer MoS2 using Inorganic Molecular Precursors

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We accomplished the synthesis of highly-orientated monolayer MoS2 on c-cut sapphire using the IVCVD system. The CVD system has been known as a method of synthesizing a large area, uniform, and high-quality TMDs. Here, we used the vapor precursors of MoOCl4 and H2S to synthesize the highly-orientated monolayer MoS2. In the CVD system, the selection of substrate is crucial to synthesize the highly-orientated monolayer MoS2. Although sapphire substrate is widely used to grow the highly-orientated monolayer MoS2, the growth mechanism of highly-orientated monolayer MoS2 on sapphire is still lacking. We have confirmed changing the contact angle of sapphire surface termination according to temperature and surface energy of sapphire with MoS2 grain was calculated using DFT to find the dependence of crystallinity of MoS2. Synthesized highly-orientated monolayer MoS2 on sapphire was confirmed using UV-Vis, XPS, Raman, PL, TEM, and so on. Because our samples observed high photoluminescence, it can advance the applications of MoS2 optoelectric devices.

Poster Presentation : **INOR.P-294**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Nanomechanical identification of Lung Cancer Extracellular Vesicles with Different EGFR Mutations by Atomic Force Microscopy

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Lung cancer has a high mortality and metastatic rate. Exosomes have been suggested as biomarkers of lung cancer. Exosomes are a 30 – 150 nm-sized subtype of extracellular vesicles (EVs) that are secreted by all cell types and are responsible for intracellular communication (between tumor and host cells). Approximately 80% of the exosomes isolated from lung cancer biopsies contain epidermal growth factor receptor (EGFR) which has the potential to lead to the suppression of tumor antigen specific CD8+ cells. EGFR is the transmembrane glycoprotein inducing cell differentiation and proliferation. Receptors are located at the cell surface, where the binding of the ligand activates a tyrosine kinase in the intracellular region. The overexpressed and mutated EGFR enables tumor cells to become independent of external growth control cues and drives persistent survival signaling.1 The plasma membrane of cancer cells has significant changes in its structure and organization to support growth factor signaling. The signaling activity of the plasma membrane is influenced by its biophysical properties, including fluidity, charge, and local architecture.2 The altered growth factor signaling mediated by the mutated EGFR can determine the levels of major lipid classes, resulting in changes of the plasma membrane composition.3 However, how the altered EGFR signaling regulates the membrane elasticity and changes the lipid raft structure are not well understood. Here, we detect and quantitatively measure the nanomechanical properties of the EGFR clustered lipid rafts in the plasma membranes of extracellular vesicles from the four types of lung cancer cells using atomic force spectroscopy (AFM). We employ anti-EGFR antibody-attached AFM probe that binds to the single-molecule EGFR to locate the EGFRs on the surface. At the same time, the AFM probe measures the elasticity of the EGFR clustered lipid rafts by applying nanoindentations. This study can identify the biophysical relationship between genetic mutations in the growth factor signaling system and

the reorganization of the plasma membrane composition.Reference1.Lin, C. C. et al. Theranostics 2020, 10, 10925-10939.2.Guéguinou, M. et al. Biochim. Biophys. Acta 2015, 1848, 2603-2620.3.Bi, J. et al. Cell Metab. 2019, 30, 525-538.e8.

Poster Presentation : **INOR.P-295**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

A Diphenyl-Substituted ^{acri}PNP Ligand Platform for CO_2 Activation

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As a key technology for the carbon neutral industry, the conversion of CO_2 into industrially important products has been of keen interest in recent years. In particular, CO_2 conversions mediated by transition metal complexes continue to attract much attention because various value-added products can be generated. Our group has explored the chemistry of low-valent nickel supported by pincer systems. We first investigated the flexible PNP ligand and reported the reaction of the zerovalent nickel complex {Na}{(PNP)Ni(CO)}, with CO_2. Due to the nucleophilicity of the central amido nitrogen of the PNP ligand, the reaction resulted in the generation of multiple products, including a tetrameric cluster complex. This suggested that competition might occur between the nickel ion and an amido nitrogen during the reaction. Recently, we also reported a new ^{acri}PNP pincer ligand (^{acri}PNP– = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide), and its nickel complexes. This rigidified (^{acri}PNP)Ni scaffold showed a unique result. Upon addition of CO_2 to the nickel(0)–CO species, a nickel(II) carboxylate species with a Ni(η1-CO_2-κC) moiety was successfully formed. This selective reaction implies that the role of the methyl groups in the ligand, in the secondary coordination sphere, play a role in suppressing the competing reaction. We further modified the PNP ligand to prepare the ^{acri}PNP^{Ph} pincer ligand, where ^{acri}PNP^{Ph}– = 4,5-bis(diisopropylphosphino)-3,6-dimethyl-9,9-diphenyl-9H-acridin-10-ide, and explored the reactivity of their low-valent nickel carbonyl species towards CO_2. We believe that the bulkier phenyl groups would provide better steric shielding of the amido nitrogen. These results will be discussed.

Poster Presentation : **INOR.P-296**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

New synthesis of highly active Rh–Co alloy nanoparticles supported on N-doped porous carbon (Rh-Co/NPC) for catalytic C–Se cross-coupling reaction

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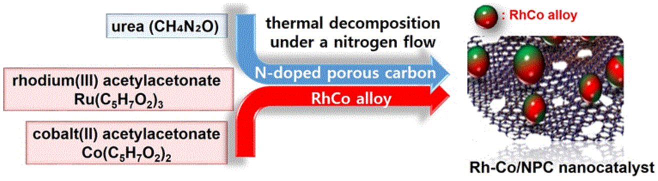
A new Rh–Co alloy nanoparticles supported on nitrogen-doped porous carbon (Rh–Co/NPC) were synthesized from metal precursors and urea using high-energy ball milling method through a simple thermal decomposition/reduction under a nitrogen flow. These nanoparticles have been developed and have gained considerable attention because of their multiple unique properties compared to those of single metal nanoparticles, such as high electronic and optical properties, selectivity, and stability. These improved properties were attributed to the combination of properties arising from two metals and the formation of new properties due to the synergistic effect of two metals. The Rh–Co/NPC nanocatalyst which contains highly dispersed alloy nanoparticles (~6 nm) showed high catalytic performance as well as good recyclability for the C–Se coupling reaction of diphenyl diselenide and aryl boronic acid, which is very useful in the biochemistry field.



Poster Presentation : **INOR.P-297**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Lewis Acid Catalysis at Switchable Open Metal Sites in MFM-300(Sc) Enabled by Dynamic Metal-Linker Bonds

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In the development of MOF (Metal-organic Frameworks) catalysis, three different methodologies have emerged to imbue MOFs with catalytically active sites: 1) post-synthetic modification (i.e. incorporating active metal sites);1 2) loading the MOF with active constituents (i.e. metallic nanoparticles (MNPs)); 3) metal ions/node being the catalytically active site. One of the most attractive approaches is the metal node to be the active site of the catalytic cycle due to the facile synthesis. These metal nodes in the MOFs often serve as potent Lewis-acid catalysts for reactions that involve metal-substrate bond formation, but the crystal structures of these MOFs typically appear coordinatively saturated. Hemilabile metal-linker bonding would explain this contradiction, although MOF bonds are generally viewed as rigid. Recently, has been reported evidence for dynamic bonding in common MOFs, suggesting that reversible metal-linker dissociation triggers important MOF behaviour. Here, we present an experimental-computational investigation of MFM-300(Sc), an unusually stable MOF with coordinatively saturated Sc (III) centres. Vibrational spectroscopy and DFT modelling indicate MFM-300(Sc) exhibits among the most dynamic metal-carboxylate bonds of a MOF. As a proof-of-concept, we demonstrate that it catalyzes a Strecker transformation, which necessitates open metal sites at Sc (III). Defects alone cannot account for this reactivity, while computations identify intermediates involving dissociated Sc-carboxylate bonds. These results highlight dynamic MOF bonding as a viable platform for designing heterogeneous catalysts with molecularly defined materials.

Poster Presentation : **INOR.P-298**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Synthesis and Characterization of New Nickel Complexes Supported by Bismuth Pincer Ligand

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Recently, developing new catalysts with high economic advantages using 1st row transition metals are drawing attention. Such 1st row transition metal complexes are not widely used in industry due to their limited applications, even though they are inexpensive and abundant. Controlling the properties of 1st row metals to mimic the intrinsic character of the frontier orbitals of heavy 2nd and 3rd row metals would expand its utility. Metal-ligand cooperation (MLC) has been employed as a new synthetic methodology to tune the chemical properties of the light transition metals. In this study, we synthesized a series of new bismuth-nickel pincer complexes supported by tetradentate ligand (BiP3) to explore the reactivity of the Bi–Ni site. From a BiP3 ligand, the oxidative-addition of a Bi–C bond at nickel(0) species gave a distorted trigonal bipyramidal nickel(II) complex, (BiP)2Ni(PPh). In the reaction with MeI, the nickel(II) complex also showed the oxiative-addition product, (BiP2Me)Ni(I)(PPh), where methylation occurs at the Bi site and nickel gets oxidized by 2-electrons. Subsequent exposure to UV-irradiation resulted in the four-coordinate reduction product, (BiP2)Ni(I), possessing highly distorted square planar geometry with a shortened Bi–Ni bond length compared to that of (BiP)2Ni(PPh). As an alternate way to prepare a metal-halide complex, HCl was directly reacted with (BiP)2Ni(PPh) to give (BiP2)NiCl. It was previously reported that tBuNC could facilitate migration of the nickel-bound moiety to the central phosphide moiety of a PP2 ligand. Accordingly, we treated (BiP2)NiCl with tert-butyl isocyanide, resulting in the formation of a trigonal bipyramidal species, {(BiP2)Ni(tBuNC)2}{Cl}. Interestingly, the chloride anion weakly interacts with bismuth, showing an unprecedently long Bi–Cl bond length of 3.16 Å, resulting in the elongation of the Bi–Ni bond. The resulting product, [(BiP2)Ni(tBuNC)2][BPh4], was synthesized by the addition of NaBPh4 to the {(BiP2)Ni(tBuNC)2}{Cl}. The product showed a shorter Bi–Ni bond length, 2.617(1) Å, than that of the starting material. This work provides information on the bonding character of two metal sites, bismuth and nickel, as well as the reactions which occur in a heterobimetallic cooperative way.

Poster Presentation : **INOR.P-299**
Inorganic Chemistry
Event Hall FRI 11:00~13:00

Synthesis of Novel Tin(II) Sulfide Complexes Containing β-Diketonate Ligand

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Tin monosulfide (SnS) materials, which are a direct band gap semiconductor, have applications in various areas such as photovoltaic solar cells, optoelectronic devices, and polymerization reactions. Especially, SnS having a high absorption coefficient ($>10^4$ cm^{-1}) and almost ideal direct band gap of ca. 1.3 eV has recently attracted considerable attention for its ability as a solar absorbent. However, the effectiveness of SnS-based photovoltaic absorber candidates is still low. Therefore, we have focused on the synthesis of new tin sulfide complexes aimed at increasing the thin film deposition efficiency by enhancing the interaction ability between the Sn central metal and the S derivative.A series of novel tin(II) precursors have been successfully synthesized using the β-diketonate and thioketone derivative ligands. These complexes were stabilized by bonding effect with each ligand. It was thought that the tin metal forms strong bonding by monoanionic *O*,*O*-chelates with β-diketonates, and *S*,*O*-chelates with thioketone ligand.All the synthesized complexes were fully characterized by NMR and FT-IR spectroscopy along with elemental analysis and thermogravimetric (TG) analysis. Newly synthesized Sn complexes have potential properties for single source precursors to prepare metal sulfide materials.

Poster Presentation : **INOR.P-300**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Characterization of New Strontium Complexes with Multidentate Ligands

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[2]*Department of Chemistry, Korea University, Korea*

Group 2 metals such as calcium, barium, and strontium, especially the latter on, are attractive elements because of their variety of applications like e.g. in optical waveguides, electrically tuneable microwave devices, colossal magnetoresistive thin films, or metal-insulator-metal (MIM) capacitors. In these fields, fabrication of thin film containing strontium oxides is required which can be deposited by various ways such as metal-organic chemical vapour deposition (MOCVD), or atomic layer deposition (ALD). To apply these deposition techniques, strontium precursors exhibiting volatility and thermal stability are essential. However, the synthesis of suitable compounds for the deposition of strontium oxides is limited due to their tendency to form oligomeric complexes which can be attributed to their large radius, small charge, and high coordination number. To prevent oligomerization, we introduced bulky and multidentate ligands. In this study, we produced heteroleptic complexes using pentadentate aminoalkoxide ligands and β diketonate ligands to prevent the formation of oligomeric complexes. The complexes, [Sr(tmtad)(btsa)]2 (1), [Sr(ptmtad)(btsa)]2 (2), [Sr(etmtad)(btsa)]2 (3), [Sr(tmtad)(tmhd)]2 (4), [Sr(ptmtad)(tmhd)]2 (5), and [Sr(etmtad)(tmhd)]2 (6) were prepared by controlled substitution reaction on strontium bis(trimethylsilyl)amides (Sr(btsa)2·2 DME). All compounds were characterized using Fourier-transform infrared spectroscopy (FT-IR), elemental analysis (EA), thermogravimetric analysis (TGA), and nuclear magnetic resonance (NMR) spectroscopy. Additionally, molecule structures of complexes 1, 3, and 6 were characterized via X-ray crystallography.

Poster Presentation : **INOR.P-301**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

Synthesis, crystal structure and thermal stability of a new proton conductor, HTa_2PO_8

Yewon Yoon, Seung-Joo Kim[*], Dayoung Lee

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Proton conducting solid-state electrolytes are important for the development of intermediate temperature (150-600℃) fuel cells. In this study, a useful protonated/deuterated compound, HTa_2PO_8 was synthesized via the ion-exchange reaction of $LiTa_2PO_8$ in aqueous HCl solution. The crystal structure of HTa_2PO_8 was determined by the complementary use of synchrotron X-rays and neutron powder diffraction. Two distinctive H^+ sites were observed in the solid-state ^1H nuclear magnetic resonance spectrum of HTa_2PO_8. Combined thermogravimetry and in-situ high temperature X-ray diffraction results show the formation of proton-free $Ta_2PO_{7.5}$ at 600℃ without any change in the framework and its subsequent decomposition to Ta_2O_5 and $TaPO_5$ above 1050℃. The results of impedance spectroscopy measurements of HTa_2PO_8 performed under dry and wet air showed that the main transporting species in HTa_2PO_8 in the protons. We expect that the aqueous ion-exchange of $LiTa_2PO_8$ will facilitate the development of cationic ion conductors involving various mobile cations. In addition, $Ta_2PO_{7.5}$ can be potentially utilized in various applications involving inorganic porous frameworks.

Poster Presentation : **INOR.P-302**

Inorganic Chemistry

Event Hall FRI 11:00~13:00

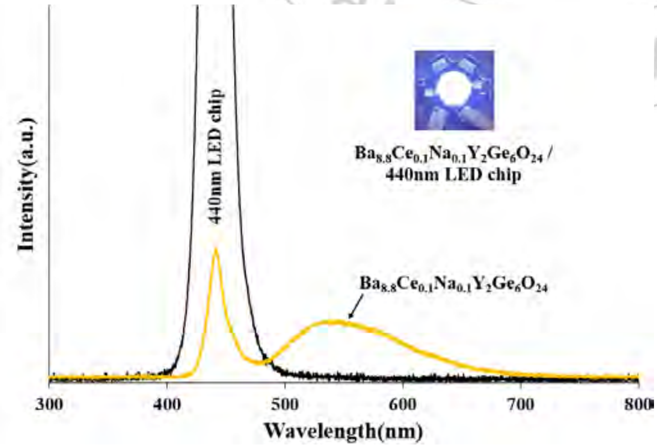
New green-yellow orthogermanate-type phosphors for white-LED

Seungyong Shin, Sungjun Yang, Sangmoon Park[1,*]

Department of Engineering in Electronics & Energy Materials, Silla University, Korea

[1]*Department of Environmental Energy & Chemistry, Silla University, Korea*

Green-yellow phosphors based on Ce^{3+}-doped barium yttrium orthogermanate host, which were synthesized by solid-state method using LiCl flux [1]. The structure and X-ray diffraction patterns were determined with the use of synchrotron X-ray powder diffraction [2]. Photoluminescence (PL) excitation and emission spectra, Gaussian deconvolution of fitting emission bands and scanning electron microscopy (SEM) images were obtained [1]. The white light with color-rendering index (CRI), correlated color temperature (CCT), Commission International de l'Eclairage (CIE) coordinates and internal quantum efficiency (IQE) were characterized for the $Ba_{8.8}Ce_{0.1}Na_{0.1}Y_2Ge_6O_{24}$ phosphor using a 440 nm LED chip [1].[Reference][1] S. Shin, S. Yang, S. Lee, T. Shin, S, Park, J. Alloys Compd. 897, 163213 (2021)[2] S. Yang, T. Shin, S. Park, J. Alloys Compd. 777, 572-577 (2019)



Poster Presentation : **INOR.P-303**

Inorganic Chemistry

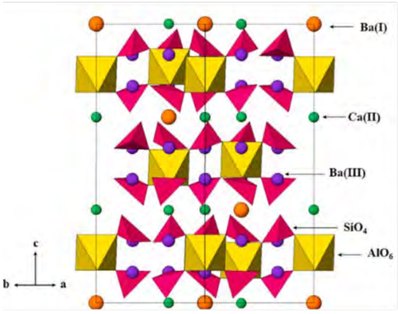
Event Hall FRI 11:00~13:00

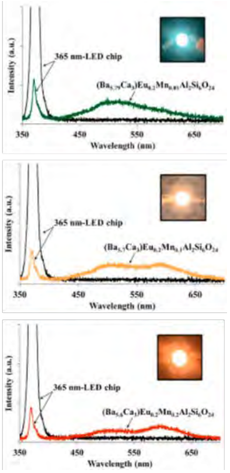
Color tunable $Ba_{9-p}Ca_pAl_2Si_6O_{24}:Eu^{2+}$, Mn^{2+} orthosilicate phosphors for NUV-LED

Sungjun Yang, **HeonJi Ha**[1], **TaeYoon Kim**[1], **Jae Hyuk Park**[2], **Sangmoon Park**[1,*]

Department of Engineering in Electronics & Energy Materials, Silla University, Korea
[1]*Department of Environmental Energy & Chemistry, Silla University, Korea*
[2]*Silla University, Korea*

Optical materials of $(Ba_{8.8-p-q}Ca_p)Eu_{0.2}Mn_qAl_2Si_6O_{24}$ (p = 2–4, q = 0–0.2) were synthesized by solid-state reactions. The photoluminescence emission spectra of the $(Ba_{8.8-p}Ca_p)Eu_{0.2}Al_2Si_6O_{24}$ phosphors depending on the Ca^{2+} ion content were exploited under 365nm excitation. When the Eu^{2+}-Mn^{2+} was co-doped in the $(Ba_{8.8-p}Ca_p)Eu_{0.2}Al_2Si_6O_{24}$ structure, the energy-transfer mechanism from Eu2+ to Mn2+ was investigated, and their electric multipole interactions were examined. Thermal quenching of the $(Ba_{8.7-p}Ca_p)Eu_{0.2}Mn_{0.1}Al_2Si_6O_{24}$ (p = 2–4) phosphors with a clear blue-shift of Mn^{2+} transitions was observed in the range from 298 to 448 K. The CIE coordinates of the green, white, and orange regions were observed in the $(Ba_{5.89}Ca_3)Eu_{0.2}Mn_{0.01}Al_2Si_6O_{24}$, $(Ba_{5.7}Ca_3)Eu_{0.2}Mn_{0.1}Al_2Si_6O_{24}$, and $(Ba_{5.6}Ca_3)Eu_{0.2}Mn_{0.2}Al_2Si_6O_{24}$ phosphors on the 365-nm LED chip. The internal quantum efficiency (IQE) of the phosphor-converted LEDs were decreased from 53 to 29% with the increase of Mn^{2+} ions.





129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-11**

Physical Chemistry

Event Hall THU 11:00~13:00

Unveiling surface structure of Fe-TiO_2 photocatalysts active for NO oxidation

HuiCheol Choe, Shufang Zhao, Miyeon Jeong, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

We used commercial rutile TiO_2 particles capped with Al_2O_3 and ZrO_2 layers, widely used as white pigment, as a starting material for the fabrication of visible light responsive photocatalysts towards gas phase NO oxidation. The as-received TiO_2 with Fe impurity showed a lower photocatalytic activity, and the activity was boosted by deposition of additional Fe comparable to the intrinsic Fe impurity level in quantity. Analyses using XPS, ToF-SIMS and LEIS revealed that the natures of additionally deposited Fe and intrinsic impurity Fe are quite dissimilar in terms of location, oxidation states and interaction with TiO_2. We highlight that tracking structure of elements in a photocatalysts with impurity level in amount can be crucial for understanding the structure-activity relationship for real catalyst.

Poster Presentation : **PHYS.P-12**

Physical Chemistry

Event Hall THU 11:00~13:00

A Novel photo-switchable hydrogel based on hyaluronate for DNA release

Yen Nguyen Thi, Namdoo Kim[1,*]

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In recent decades, hydrogels have been extensively investigated as a model platform for drug delivery and controlled release due to their distinctive properties such as swollen controllable, biocompatible and bio-mimetic. Among the others, the environmental-adaptive hydrogels have received a great attention since they have been revealed to change their physiochemical properties and phase states rabidly and controllably toward the versatile stimulations. The photo-responsive hydrogel, which has been of a great interest among those environmental-adaptive hydrogels, has opened a new approach for studying drug delivery. Herein, we introduce a new hydrogel platform for drug delivery based on maleimide functionalized hyaluronic acid (HA-Mal), crosslinked by photo-dissociable dimeric Dronpa green fluorescence protein (pdDronpa). This hydrogel was formed by the Michael-type addition reaction, through the conjugation of maleimide groups bearing on HA chains with the free cysteine sites of pdDronpa. The results demonstrated that the pdDronpa-HA-Mal hydrogel was reversibly and rapidly switched its states between sol and gel upon 500 nm and 400 nm illumination, as a result of the photo-dissociation and re-association of pdDronpa between dimeric and monomeric forms. The response behaviors of the Dronpa-HA-Mal hydrogel to photo-stimulation were further evidenced by SEM imaging and rheological performs, indicating the disintegration and aggression of the crosslinked network of the hydrogel toward 500 nm and 400 nm illumination. Besides, the photo-controlled release of DNA was also investigated using this hydrogel platform, showing the release of DNA from the hydrogel can be simply controlled by adjusting the dose of pdDronpa and illuminations.

Poster Presentation : **PHYS.P-13**

Physical Chemistry

Event Hall THU 11:00~13:00

Solvolysis Mechanism Change of Benzoyl Chlorides According to Trifluoromethyl Substituents

Seoyeon Jang, ChanJoo Rhu[1], GilHoon Kim[2], Kyoungho Park[2,*], Hoshik Won[3], Jin Burm Kyong[3], Dennis N. Kevill[4,*]

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[1] *Enviromental Testing Center, Korea Conformity Laboratories, Korea*
[2] *Department of Chemical and Molecular Engineering, Hanyang University, Korea*
[3] *Department of Applied Chemistry, Hanyang University, Korea*
[4] *Chemistry and Biochemistry, Northern Illinois University, United States*

The solvolysis mechanism of 2,5-bis(trifluoromethyl)benzoyl chloride(**1**) was revealed by conductivity methods at 25.0 ^{o}C. The comparison with the results of benzoyl chloride(**2**) and 2-trifluoromethyl benzoyl chloride(**3**) was able to illustrate the effects of the trifluoromethyl substituent on the solvolysis mechanism. These effects were considered from the structural and inductive effect of substituent. At first, it was resulted that **1** is followed the addition-elimination(A-E) mechanism on all solvents. The extended Grunwald-Winstein equation was resulted 1.56 ± 0.15 of *l*, 0.42 ± 0.08 of *m*, and 0.960 of R(correlation coefficient), and the kinetic solvent isotope effect(KSIE) was obtained 2.30 which is a usual value for A-E mechanism. The activation parameters, also, were obtained that $\Delta H^{\neq}$ = 11.0 ~ 16.2 kcal/mol and $\Delta S^{\neq}$ = -31.8 ~ -21.7 cal/mol·K in the selected solvents at various temperatures. The above contents were pointed at that **1** is governed the bimolecular reaction, specially the addition-elimination mechanism what has the tetrahedral structure as a transition state. **2** has a flat structure that benzene and acyl chloride group were the same plane. **3** has a vertical structure of benzene and acyl chloride group because of *ortho*-substituent. Although **1** has the same structure as **3**, the results was that was followed the different mechanism, because **1** has another trifluoromethyl substituent at *meta*-site. This substituent affect the lack of electron density on reaction center of carbonyl carbon, so the mechanism of **1** is effected by a structural factor and an inductive effect along site and kind of substituent.

Poster Presentation : **PHYS.P-14**

Physical Chemistry

Event Hall THU 11:00~13:00

Competitive S_1 decay channels in halophenols: Role of intramolecular hydrogen bonding on the relaxation dynamics

Junggil Kim, Kyung Chul Woo[1], Minseok Kang, Sang Kyu Kim[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Division of Chemistry and Biological Chemistry, Nanyang Technology University, Singapore*

The S_1 state relaxation dynamics of *ortho*-chlorophenol derivatives has been investigated using picosecond pump-probe spectroscopy. Here, H/D primary kinetic isotope effect (KIE) has been also measured to determine the yield of H(D) atom tunneling pathway. In contrast to the phenol which undergoes H atom dissociation via tunneling as a major dissipation channel on the S_1 state, for *ortho*-chlorophenols, it has been found that another relaxation pathways are competing with the tunneling even at their zero-point energy level. For instance, the S_1 lifetimes of *ortho*-chlorophenol is found to be ultrashort with KIE = 1 within a picosecond, implying that the tunneling in this case is suppressed by another competitive dynamic channel. The statistical product ratio $\Phi(H)/\Phi(D) \sim 4$ after dissociation of deuterated *ortho*-chlorophenol suggests that the S_1 population may undergo nonradiative decay from the internally hot S_0 state via S_1/S_0 conical intersection generated by the O-H···Cl intramolecular hydrogen bonding coordinate. *Ab initio* excited state calculations regarding the $S_1(\pi\pi^*)$ and $S_2(\pi\sigma^*)$ states on the C-Cl bond length coordiniate well support our experimental observations.

Poster Presentation : **PHYS.P-15**

Physical Chemistry

Event Hall THU 11:00~13:00

Atomic-level Thermodynamic Analysis of the Binding Free Energy of SARS-CoV-2 Neutralizing Antibodies

Jihyeon Lee, Song-Ho Chong[1], Chaok Seok[2,*]

department of chemistry, Seoul National University, Korea
[1]*RIKEN BDR, Japan*
[2]*Division of Chemistry, Seoul National University, Korea*

The global health crisis caused by the coronavirus disease (COVID-19) is on-going, and effective treatments have yet to be developed to end the pandemic. Atomistic understanding of the binding mechanism of neutralizing antibodies to the target antigen, the receptor-binding domain (RBD) of the SARS-CoV-2 spike protein, is a key ingredient for developing effective treatments. Here, we investigate the binding free energy of antibodies to RBD at an atomistic level by applying the site-directed thermodynamics analysis to simulated antibody-RBD complexes. This quantitative analysis reveals that simultaneous formation of hydrogen bonds and hydrophobic contacts between antibody and RBD play a critical role in gaining favorable binding free energy. The insights obtained by this study will shed new light on our understanding of binding between antibody and antigen and on designing new effective antibodies for the current and future health emergencies.

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Poster Presentation : **PHYS.P-16**

Physical Chemistry

Event Hall THU 11:00~13:00

Intersystem Crossing and Vibrational Autodetachment Dynamics on Dipole-bound state in deprotonated 4,4’-biphenyl anion

Jinwoo Kim, Do Hyung Kang, HanJun Eun, Sang Kyu Kim*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Dipole-bound state (DBS) has been recently spotlighted as ‘doorway state’ to form the anionic species in nature. Despite its importance, the observation of the definitive evidence of non-adiabatic coupling between the DBS and valence-bound state in experiment has been scarcely reported up to date. Here, we firstly observed the intersystem crossing (ISC) dynamics on DBS into the valence-bound triplet state in deprotonated 4,4'-biphenyl anion (bPh^-) by employing the picosecond time-resolved spectroscopy combined with a cryogenically-cooled Paul ion trap. The ISC lifetime was measured to be ~5 ns and barely influenced on the vibration modes of DBS. Above the detachment threshold, autodetachment dynamics of vibrational Feshbach resonances were thoroughly investigated, which is found to be shorter than prediction in Fermi's golden rule. This may originate from the effect of intramolecular vibrational redistribution (IVR), smearing out the mode-characters of the DBS within tens of picosecond time scale. The non-adiabatic relaxation dynamics explains DBS serves as ‘doorway state’ in nature, such as anion formation in the interstellar medium or robustness of DNA against the slow electron-induced damage.

Poster Presentation : **PHYS.P-17**

Physical Chemistry

Event Hall THU 11:00~13:00

Tracking Multiexcitonic Triplet Pair Dynamics via Time-Resolved Magneto-Optical Spectroscopy

Juno Kim, Dongho Kim[*]

Department of Chemistry, Yonsei University, Korea

A spin manifold of multiexcitonic triplet pair state consists of nine spin configurations including one singlet, three triplet and five quintet spin states. A primary multiexciton state born from singlet exciton fission dynamics manifests spin singlet character, which accounts for its ultrafast dynamic nature contrary to inefficient intersystem crossing process via spin-orbit coupling. Though, the existence of quintet triplet pair states was proposed as a key intermediate state to generate two individual triplet excitons based on time-resolved electron paramagnetic resonance measurements. TR-EPR spectra suggested that quintet signal decays as triplet signatures become manifested, which is further verified by spin-echo experiments. As such, exploration of spin states in multiexcitonic triplet pair states has been a emerging issue to understand the mechanism of free triplet generation process. In this study, time-resolved magneto-optical measurements were conducted on linear and dendritic TIPS-tetracene structures to understand spin dynamics of multiexcitonic triplet pair state. In favor of qualitative singlet exciton fission processes in TIPS-tetracene structures, multiexcitonic triplet pair dynamics are investigated in terms of interchromophore couplings which originates from their structural characteristics such as choromophore orientation, interchromophoric distance and molecular flexibility. In addition to the merit from our targeted structures, time-resolved magneto-optical spectroscopy offers superior time-resolution to track spin dynamics which was hindered in TR-EPR measurements. Spin dynamics of multiexcitonic triplet pair state governs its recombination and dissociation dynamics which are key for making use of doubled triplet excitons.

Poster Presentation : **PHYS.P-18**

Physical Chemistry

Event Hall THU 11:00~13:00

Electronic Structure of a Nickel Compound that Features a Phosphine-Substituted Bis(imino)pyridine Chelate - An MCSCF Study

Jun-Hyeong Kim, Ryan J. Trovitch[1], Mu-Hyun Baik*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*School of Molecular Sciences, Arizona State University, United States*

It was recently discovered that (Ph2PPrPDI)Mn adopts the doublet ground state with Mn(II)-PDI2– assignment where unpaired electrons on Mn(II) center are antiferromagnetically coupled to PDI-based unpaired electrons. The most interesting aspect of (Ph2PPrPDI)Mn is that it is the most efficient manganese-based hydrosilylation catalyst to date. Inspired by previous work, we were interested in elucidating electronic structure of a series of late base-metal complexes (Ph2PPrPDI)M (M = Fe, Co, and Ni), and their catalytic activity on carbonyl hydrosilylation. Among these, (Ph2PPrPDI)Ni draws much attention as our preliminary density functional calculations are in sharp contrast with the experimental data, e.g. EPR spectra, structure, and oxidation state. Not only this, (Ph2PPrPDI)Ni was found to exhibit a solution magnetic moment of 1.23 μB at 25 °C, which is lower than spin-only values of singlet and triplet states. Furthermore, while (broken-symmetry) density functional theory becomes a standard tool of understanding chemical reactivity and electronic structure of a given complex, it provides unrealistic solutions when strong nondynamic correlation dominates in the system of interest. Using multiconfigurational approach of complete active space that is a state-of art tool of studying strongly correlated systems where density functional theory breaks down, I provide a detailed computational study on (Ph2PPrPDI)Ni in order to address the questions above.

Poster Presentation : **PHYS.P-19**

Physical Chemistry

Event Hall THU 11:00~13:00

Determining the charge distribution and the direction of bond cleavage with femtosecond anisotropic x-ray liquidography

Jun Heo, Hyotcherl Ihee[1,*]

Department of chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Energy, structure, and charge are fundamental quantities characterizing a molecule. Whereas the energy flow and structure change in chemical reactions are experimentally characterized, determining the atomic charges of a molecule in solution has been elusive, even for a triatomic molecule such as triiodide ion, I_3^-. Moreover, it remains to be answered how the charge distribution is coupled to the molecular geometry; which I-I bond, if two I-I bonds are unequal, dissociates depending on the electronic state. Here, femtosecond anisotropic x-ray solution scattering allows us to provide the following answers in addition to the overall rich structural dynamics. The analysis unravels that the negative charge of I_3^- is highly localized on the terminal iodine atom forming the longer bond with the central iodine atom, and the shorter I-I bond dissociates in the excited state, whereas the longer one in the ground state. We anticipate that this work may open a new avenue for studying the atomic charge distribution of molecules in solution and taking advantage of orientational information in anisotropic scattering data for solution-phase structural dynamics.

Poster Presentation : **PHYS.P-20**

Physical Chemistry

Event Hall THU 11:00~13:00

Enhancing photoelectrochemical activity of Bismuth vanadate with Silver Plasmonic Nanoparticles as Photosensitizers and Cobalt phosphate as Oxygen evolution catalyst

Kethireddy Arun Joshi Reddy, Praveen Kumar Dharani[1], Tae Kyu Kim[1,*]

Chemistry, Yonsei University, Korea
[1]*Department of Chemistry, Yonsei University, Korea*

Solar-driven photoelectrochemical (PEC) water splitting is a promising and environmentally friendly route for the conversion of solar energy into useful fuels. Sufficient visible light harvesting, as well as separation and transport of photogenerated charges, play a pivotal role on the photoelectrochemical performance of photoelectrodes. Bismuth vanadate ($BiVO_4$) has shown great potential for PEC catalysis, but it needs to be further modified because of its inadequate light harvesting, charge separation and transfer efficiencies have harshly limited the photoelectrochemical water oxidation performance. Herein, we modified $BiVO_4$ photoanode by plasmonic Silver (Ag) nanoparticles and with cobalt phosphate (Co-Pi) to accomplish effective water splitting. In this $BiVO_4$/Ag/Co-Pi photoanode, the Ag nanoparticles acts as photosensitizers broaden the absorption spectrum and promote charge separation due to its enchanting surface plasmon resonance effect, moreover Co-Pi acts as hole transfer layer which stimulate charge separation and transfer and enhance the stability of photoanode. As a result, the $BiVO_4$/Ag/Co-Pi photoanode generates enhanced photocurrent at 1.23 V (vs RHE) under 1.5G illumination in 0.5M Na_2SO_4 electrolyte solution, which is virtually 5 times higher than that of bare $BiVO_4$. The surface modification approach developed in this work remarkably promotes the photocurrent density of $BiVO_4$ by facilitating carrier transfer in addition to a charge separation efficiency enhancement.

Poster Presentation : **PHYS.P-21**

Physical Chemistry

Event Hall THU 11:00~13:00

How the point mutation of NPC1 can affect the cholesterol transport efficiency: Molecular dynamics study

Hyejin Yoon, Soonmin Jang[1,*]

Department of Chemistry, Seoul National University, Korea
[1]*Department of Chemistry, Sejong University, Korea*

The NPC1 (Niemann-Pick type C1) is one of the main players of cholesterol control in the lysosome and almost its action is closed combined with NPC2 (Niemann-Pick type C2) protein. The dysfunction of one of the proteins can cause problems in overal chloesterol homestasis and leads to a disease, called the Niemann-Pick type C (NPC) disease. It has been reported that many mutations are responsible to the disease. The point mutation R518W or R518Q on the NPC1 is one of such examples. Even though many details on the cholesterol transport mechanism of NPC1 is elucidated especially with the full-length NPC1 structure obtained from cryo-EM study, it is not obvious how the simple mutation can lead such a big difference in proper function of NPC1. In this respect, the single mutation mentioned above could be a good candidate to relate the dynamical function of NPC1 to its structure in cholesterol transport.In this presentation, we report how the corresponding mutation can induces the structural change in NPC1 by molecular dynamics simulations. Detailed analysis of the resulting simulation trajectory reveals important structural features that is essential for proper function of the NPC1 for cholesterol transport. It has been found that the mutation leads to structural change that is required for proper interaction with NPC2. The current study can provide some insights into how the structure is closed related to the function of NPC1 in cholesterol transport in terms of its interaction with NPC2 protein.Funding information: This research was supported by the NRF grant funded by the Korean government (2021R1A2C1004388) and by the National Supercomputing Center with supercomputing resources including technical support (KSC-2021-CRE-0253) to HJY.

Poster Presentation : **PHYS.P-22**
Physical Chemistry
Event Hall THU 11:00~13:00

Small Charged Biomolecules in FUS Protein Aggregation

Hyeryeong Lee[*], Sang Hak Lee[*]

Department of Chemistry, Pusan National University, Korea

FUS protein aggregation is the main cause of amyotrophic lateral sclerosis (ALS), one of the neurodegenerative diseases. It is known that the low complexity domain (LCD) of FUS, which has 214 amino acid residues, mainly contributes to making protein aggregation in cells. Since the LCD is an intrinsically disordered domain, it does not have a specific structure but just a random coil. Thus, it is easy to be aggregated through molecular interaction. In addition, the LCD domain is highly negatively charged (-14 e) at the physiological condition. Therefore, we thought that the multivalent cation is necessary to create the aggregation of the LCD. Metal ions, such as Mg2+ and Ca2+, can be good candidates to make protein aggregates; however, the size of metal ions is too small to mediate the interaction between proteins. Thus, we were interested in investigating multivalent small biomolecules, in particular polyamine molecules. Therefore, we made the plasmid to express the LCD with dronpa3 (analog of green fluorescence protein) in cells. We found that the LCD aggregated when adding polyamine molecules to cells. In order to clarify the results, we compared two different types of E-coli strains: BL21 and HT873. Since the HT873 strain does not create endogenous polyamine molecules, we could not see aggregation before adding polyamine. After adding polyamine to the media, we were able to see more drastic changes in protein aggregation in the HT873 strain than BL21. We came to the conclusion that polyamine molecules, multivalent small cationic molecules, are mainly attributed to the FUS aggregation in cells.

Poster Presentation : **PHYS.P-23**

Physical Chemistry

Event Hall THU 11:00~13:00

[Withdrawal] Effect of the abolition of intersubunit salt bridges on allosteric protein structural dynamics

Minseo Choi, Hyotcherl Ihee*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

129th General Meeting of the Korean Chemical Society
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Poster Presentation : **PHYS.P-24**

Physical Chemistry

Event Hall THU 11:00~13:00

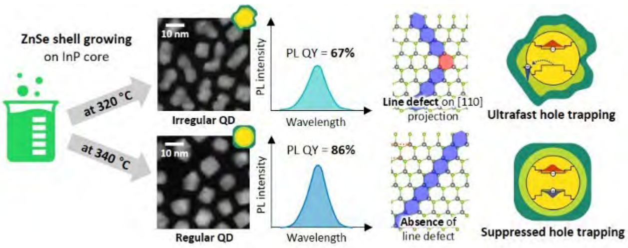
Spectroscopic Insight into High Efficiency of Isotropic InP/ZnSe/ZnS Quantum Dots

Jumi Park, Dongho Kim[1,*]

Yonsei University, Korea

[1]*Department of Chemistry, Yonsei University, Korea*

In this study, we propose a strategy to increase the luminescence efficiency in eco-friendly InP QDs. When synthesizing InP/ZnSe/ZnS QDs, we manipulated the shell growth rates by controlling the ZnSe shell growth temperature. In a pristine synthesis of InP/ZnSe/ZnS QDs, ZnSe shell growing was conducted at 320 °C and these QDs exhibit irregular shell shape. Isotropic InP/ZnSe/ZnS quantum dots (QDs) are prepared at a high reaction temperature (340 °C), which facilitates ZnSe shell growth on random facets of the InP core. Fast crystal growth enables stacking faults elimination, which induces anisotropic growth, and as a result, improves the photoluminescence quantum yield (PL QY) by nearly 20%. HR-STEM images display that the InP/ZnSe/ZnS QDs with irregular shell have considerable stacking faults and twin defects. On the contrary, isotropic QDs present a well-ordered crystalline structure and good structural quality without stacking faults. To investigate the effect of the QD morphology on photophysical properties, the PL blinking and ultrafast charge carrier dynamics were analyzed. Time- and space-resolved PL measurements show that the charge trapping significantly decreases in isotropic QDs. The excitation energy-dependent transient absorption kinetics reveals that hot hole trapping is considerably suppressed in isotropic InP QDs. These results highlight that shape-dependent PL QYs are ascribed to the degree of the hole trapping. The tactic, growing the ZnSe shell fast at the elevated reaction temperature, significantly reduced the hole trapping and improved the PL QY of InP/ZnSe/ZnS QDs. Our findings shed light on the correlation between QD shapes and hot carrier dynamics, and present a way to design highly luminescent QDs for further promising display applications.


ZnSe shell growing
on InP core
at 320 °C
at 340 °C
10 nm
Irregular QD
10 nm
Regular QD
PL intensity
PL QY = 67%
Wavelength
PL intensity
PL QY = 86%
Wavelength
Line defect on [110]
projection
Absence of
line defect
Ultrafast hole trapping
Suppressed hole trapping

Poster Presentation : **PHYS.P-25**

Physical Chemistry

Event Hall THU 11:00~13:00

The Structural Origin of the Electron Affinity of Poly-Aromatic Hydrocarbon Molecules

Jinmin Lee, Sang Hak Lee[1,*]

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[1]*Department of Chemistry, Pusan National University, Korea*

Poly-Aromatic Hydrocarbon (PAH) molecules are composed of multiple aromatic rings and are regarded as fundamental materials of graphene. In the study, we seek to understand electron affinity (EA) as the basic molecular properties of PAH molecules, to determine the electrical property of graphene. In general, the EA of linear PAH molecules increases as a function of the number of aromatic rings: naphthalene (-0.19 eV), anthracene (0.54 eV), and tetracene (1.05 eV). Having said that, phenanthrene (0.13 eV), even though the molecular formula is the same as anthracene (0.54 eV), has a different EA. Thus, we theoretically investigate the tendency of EA of larger PAH molecules using density functional theory (DFT). We found that the EA values of PAH molecules depend on the length (number of aromatic rings) of the longest acene in the molecule. Furthermore, we found that, when increasing the number of aromatic rings of the PAH molecules, the reaction position with butadiene in PAH molecules is a critical factor to determine EA values of the PAH molecules.

Poster Presentation : **PHYS.P-26**

Physical Chemistry

Event Hall THU 11:00~13:00

SERS based monitoring of photodegradation process of 2,4-dinitrotoluene by Fe_3O_4@TiO_2-Au Nanoparticles

Sila Jin, Eungyeong Park, Shuang Guo, Ah-hyun Woo[1], Yeonju Park[2], Lei Chen*, Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea
[1] *Chemistry, Kangwon National University, Korea*
[2] *Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

By decorating Au nanoparticles (NPs) on Fe_3O_4@TiO_2 NPs, it has surface-enhanced Raman scattering (SERS) activity as well as photocatalytic activity in the visible light region. Au-decorated Fe_3O_4@TiO_2 NPs (Fe_3O_4@TiO_2-Au NPs) were successfully fabricated and have photoresponse under sunlight simulated Xe lamp. The photodegradation process of 2,4-DNT by Fe_3O_4@TiO_2-Au NPs was monitored by surface-enhance Raman scattering (SERS). To deeper understand the photodegradation mechanism of 2,4-DNT, two-dimensional correlation spectroscopy (2D-COS) was applied to the SERS spectra. 2D-COS provides important information which is hardly detected in conventional 1D SERS spectra and determines the sequential order of the band intensity changes. In this study, photodegradation of 2,4-DNT under Xe lamp irradiation was monitored by SERS and UV-Vis spectroscopy and analyzed by 2D-COS. Details on its characterization and analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-27**

Physical Chemistry

Event Hall THU 11:00~13:00

Detection of Lactate by Enzyme Reaction using Surface-enhanced Raman Scattering

Eungyeong Park, Sila Jin, Hae-jin Chung[1], Hyejin Chang[2,*], Young Mee Jung[*]

Department of Chemistry, Kangwon National University, Korea
[1]*Chemistry, Kangwon National University, Korea*
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L-Lactate can be a key indicator of bioprocessing and clinical diagnostics and so on. At a high level of lactate concentration, it can reveal the phenomenon of a tumor, cardiogenic shocks, or spoilage. Surface-enhanced Raman scattering (SERS) has a lot of advantages such as obtaining the fingerprint information of molecules, identifying targets in mixtures, and detecting the target with very low concentration. For sensitively and selectively detecting the lactate, we used the SERS method. In this study, silver nanoparticles (AgNP@LOx) functionalzed with a SERS reporter (4-mercaptobenzoic acid, 4MBA)-combined with lactate oxidase (LOx) were fabricated. As the enzyme reaction occured, the SERS spectrum of 4MBA changed from the initial spectrum due to the change of polarizability. We can detect the lactate as low as 10^{-7} M.

Poster Presentation : **PHYS.P-28**

Physical Chemistry

Event Hall THU 11:00~13:00

Effect of conductivity and SERS activity of organic semiconductor PEDOT:PSS by temperature-mediated microstructural changes

Shuang Guo, Eungyeong Park, Sila Jin, Lei Chen, Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea

In recent years, organic semiconductors have provided more possibilities for improving SERS activity based on the charge transfer due to their multi-specific properties. In particular, the π-π coupling is formed by the organic semiconductor itself and between organic semiconductors and adsorbed molecules. Based on this property, we used a compound semiconductor, poly(3,4-ethylenedioxythiophen):poly(styrene sulfonate) (PEDOT:PSS), as a SERS substrate and controlled the microstructure and the molecular crystallinity by adjusting the temperature during the synthesis process. Based on results of Raman, IR, XRD, and simulation methods, the specific changes of molecular crystallinity at different temperatures were studied. The effect of this change on the conductivity and SERS activity was then analyzed. This research is expected to provide more solutions to the problem of organic semiconductors-based optoelectronic devices based on SERS research methods. The details of the mechanism will be discussed in this presentation.

Poster Presentation : **PHYS.P-29**

Physical Chemistry

Event Hall THU 11:00~13:00

Study on Charge Transfer Enhancement Mechnisum based on Carrier Density Modulating

Lei Chen, Shuang Guo, Eungyeong Park, Sila Jin, Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea

Previous study has confirmed that the charge transfer (CT) process between the materials and probe molecules. However, the effect of internal changes in materials on the CT process has not been clearly understood. Thus, modulating the effect of carrier density of materials will be a good explanation for the effect on the CT enhancement mechanism. Herein, we designed the Ag/semiconductor composite films by dual target cosputtering. The carrier density can be controlled by adjusting the content of doped elements. We found the prepared composite films show a selective SERS enhancement ability. With different characterization results, the CT process was verified by analyzing surface-enhanced Raman scattering (SERS) spectra, and the degree of CT (ρCT) was found to change synchronously with the carrier density. This study provides the new insight into control the CT by modulating of the carrier density of Ag/semiconductor composite films. In particular, the understanding of the properties of Ag/semiconductor composite films with tunable carrier density can provide in a wide range of applications, from displays and smart windows to even bioelectronic devices.

Poster Presentation : **PHYS.P-30**

Physical Chemistry

Event Hall THU 11:00~13:00

Steering the Multiexciton Generation in Slip-Stacked Perylene Bisimide Stack via Exciton Coupling

Yongseok Hong, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Understanding the structure-property relationship of organic semiconductors has been decisive to establish the design principles for ideal optoelectronic devices. Especially, despite of the extensive studies in dimer model systems and solid-state materials, the design of the game challenging material in the singlet fission (SF) field has not been accomplished so far. Here, we present a slip-stacked perylene bisimide trimer, which is a bridge between hitherto studied dimer and solid film, to investigate the multiexciton generation mechanisms. This work showcases multiple pathways towards the multiexciton state through direct or excimer-mediated mechanisms by tuning the excitation-wavelength as well as CT energy. These results suggest the comprehensive role of the exciton coupling, exciton delocalization, and excimer state to facilitate the multiexciton generation process. In this regard, our observations should expand the fundamental understanding of the SF mechanism as well as the structure-property relationship in PBIs.

Poster Presentation : **PHYS.P-31**

Physical Chemistry

Event Hall THU 11:00~13:00

Isolated Ni Single Atoms Implanted onto N-Doped Mesoporous Carbon Nanofibers for Efficient CO_2 Reduction

Yaeeun Eom

Department of Chemistry, Yonsei University, Korea

As the concentration of CO_2 in the atmosphere has reached unacceptably high levels and continues to increase, capturing CO_2 in the atmosphere and converting it to useful chemicals such as carbon monoxide, formic acid, and methane is requisite research. The strategy that reducing CO_2 to useful industrial chemicals using electrochemical CO_2 reduction powered by renewable electricity is a noteworthy approach. However, CO_2 is a stable molecule that requires high energy input to break the C=O bonds. Improving efficiencies in electrocatalytic CO_2 reduction (ECR) platforms is needed. In this regard, single-atom catalysts (SACs) are emerging catalysts for enhancing ECR reaction, and employing SACs is a promising approach to reduce catalyst cost and enhance catalytic performance. By choosing the right supports and tuning the shape of the support materials, SACs with high mass loading of single atoms without aggregation can be synthesized. Taking these factors into account, we synthesized a mesoporous Ni single atom anchored on N-doped carbon nanofiber (Ni-NCF) and evaluated the corresponding electrochemical CO_2 reduction activity. The optimized mesoporous Ni-NCF catalysts achieved a FE_{CO} value of 96.5% at -0.7 V vs. RHE. Furthermore, we can assume that the presence of remarkable morphology with high surface area influences the CO_2RR activity.

Poster Presentation : **PHYS.P-32**

Physical Chemistry

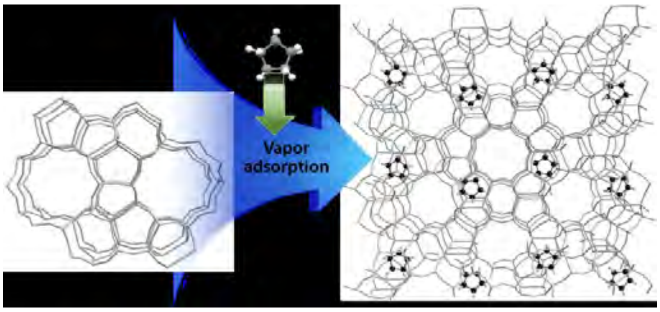
Event Hall THU 11:00~13:00

Crystallographic Study of a Cyclopentane Sorption Complex of fully Dehydrated H-ZSM-5(Si/Al = 24)

Hu Sik Kim, Hyeon Uk Choo, Ho Yeon Yoo, Woo taik Lim*

Department of Applied Chemistry, Andong National University, Korea

Zeolite Socony Mobil-5 (ZSM-5) is the highly siliceous aluminosilicate zeolite which belongs to the pentasil family of zeolite (framework type MFI from ZSM-5). ZSM-5 is renowned acid catalyst and adsorbent for its remarkable use in petrochemical industry and environmental industry. To study the cyclopentane sorption sites and the effect of sorption on the H-ZSM-5 structure, crystal of H-ZSM-5 were prepared by burning out the tetrapropylammonium cations in air. For the adsorption of cyclopentane into H-ZSM-5 crystal, the crystal was treated with zeolitically dried cyclopentane for 6 h at 297 K, and then evacuated for 600 s at this temperature and 1.1×10^{-4} Pa. The structure of a single crystal of cyclopentane sorption complex of dehydrated H-ZSM-5 (MFI, $|H_{3.8}(C_5H_{10})_{1.47}|[Al_{3.8}Si_{92.2}O_{192}]$-MFI, Si/Al = 24) has been determined crystallographically using synchrotron X-radiation in the orthorhombic space group Pnma; a = 20.141(4), b = 19.944(4), c = 13.439(3) Å. It was refined using all intensities to the final error indice R_1 = 0.072. The 1.47 cyclopentane molecules per unit cell are located between 5-rings in zigzag channel. The cyclopentane molecules are located perpendicular to the 10-rings of zigzag channel and parallel to the 5-rings of H-ZSM-5 framework at the center of them. Each cyclopentane molecule is held in place by 16 hydrogen bonds between all hydrogen atoms of cyclopentane and framework oxygen atoms of its 5- and 10-rings: C···O *ca*. 3.318 ~ 3.992 Å.



Poster Presentation : **PHYS.P-33**

Physical Chemistry

Event Hall THU 11:00~13:00

Photodissociation Dynamics of CF_2BrCF_2I in Solution Investigated by Time-resolved Infrared Spectroscopy

Seongchul Park, Manho Lim*

Department of Chemistry, Pusan National University, Korea

We investigated the photodissociation dynamics of CF2BrCF2I in CCl4 solvent excited by 267 nm energy over a broad time range from 0.3 ps to 10 μs using TRIR spectroscopy. With the support of DTF calculation results and Ar matrix experimental results, all transient absorptions in the TRIR spectra could be assigned. Most of the initially produced radicals were CF2BrCF2 radicals, and 33% of *anti*-CF2BrCF2 and 49% of *gauche*-CF2BrCF2 were produced. Also, a small amount (18%) of *anti*-CF2ICF2 were formed, unlike the gas phase experiment. *Gauche*-CF2BrCF2 were isomerized with the time constant of 47 ± 5 ps to form *anti*-CF2BrCF2. After that, *anti*-CF2BrCF2 underwent a bimolecular reaction to form CF2BrCF2Br or CF2CF2, or through a bimolecular reaction with the remaining Br atoms to form CF2BrCF2Br. All the bimolecular reactions were measured as the diffusion-limited rate constant of 6.5×10^{10} M^{-1} s^{-1} in CCl4. Secondary dissociation of *anti*-CF2BrCF2 was not observed. The remaining *anti*-CF2ICF2 underwent secondary elimination of I atom with the time constant of 60 ± 5 ns to form CF2CF2. The final products were determined to contain 50% of CF2BrCF2Br and 50% of CF2CF2. Due to the advantage of TRIR spectrometer, which is sensitive to the structure of the chemicals, for the first time, real-time dynamics between stereoisomers of CF2BrCF2 radicals could be observed. Comparison with the halo-radicals produced in the gas phase and in other parent molecules, it can be seen that the solvent can create a new reaction pathway with the dissociated halogen atom.

Poster Presentation : **PHYS.P-34**

Physical Chemistry

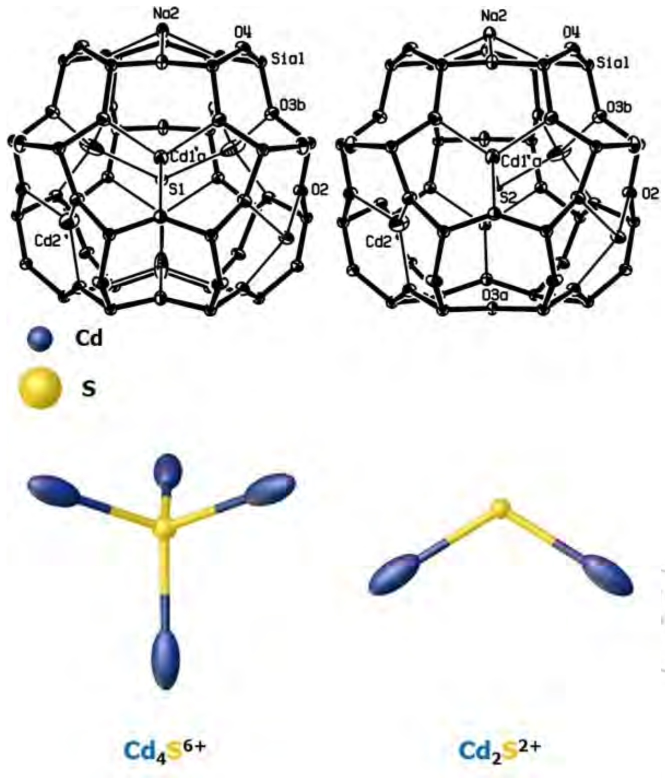
Event Hall THU 11:00~13:00

Crystal Structure of Cadmium Sulfide Cationic Cluster in Zeolite Y (FAU, Si/Al = 1.56)

Dae Jun Moon, Hu Sik Kim, Hyeon Uk Choo, Ho Yeon Yoo, Woo taik Lim*

Department of Applied Chemistry, Andong National University, Korea

The Cd_4S^{6+} and Cd_2S^{2+} clusters in the sodalite cavities were synthesized by reaction of the fully Cd^{2+}-exchanged zeolite Y (Si/Al = 1.56) and 0.1 M Na_2S(aq) solution at 294 K for 2 days. The single-crystal structure was determined at 100(1) K by synchrotron X-ray diffraction techniques in the cubic space group Fd-3m. The structure was refined using all intensities to the final error index $R_1/wR_2 = 0.048/0.156$ (for $F_o > 4\sigma(F_o)$). Approximately 13 Cd^{2+} and 53 Na^+ ions per unit cell were found at two and four crystallographically distinct positions, respectively: two site-I' positions (in the sodalite cavities opposite double 6-rings (D6Rs)) are occupied by 5 and 7.5 Cd^{2+} ions, respectively, per unit cell. The 0.5 Cd^{2+} ions per unit cell are at site II' in the sodalite cavity. The 2 Na^+ ion is located at the center of the D6R (site I). The 15.5 Na^+ ions per unit cell are located at site I'. Site-II position is occupied by 31.5 Na^+ ions per unit cell. The remaining 4 Na^+ ions per unit cell are located at sites III' near triple 4-rings in the supercage. Finally, 0.5 and 1.5 S^{2-} ions per unit cell, associated with Cd^{2+} ions, were found at the center of sodalite cavity and opposite 6-ring in the sodalite cavity, respectively. The 1 S^{2-} ion at the center of the sodalite cavity is coordinated to 4 Cd^{2+} ions at site I' to give a centered-tetrahedral cationic cluster, Cd_4S^{6+}, and the other S^{2-} ion opposite 6-ring in the sodalite cavity bridges between two Cd^{2+} ions at site I' to give a cationic cluster with a bent arrangement, Cd_2S^{2+}, in 6.3% and 18.8% of the sodalite cavities of zeolite Y (Si/Al = 1.56), respectively.


Na2
O4
Sia1
O3b
Cd1'
a
S1
O2
Cd2'
Na2
O4
Sia1
O3b
Cd1'
a
S2
O2
Cd2'
O3a
Cd
S
Cd_4S^{6+}
Cd_2S^{2+}

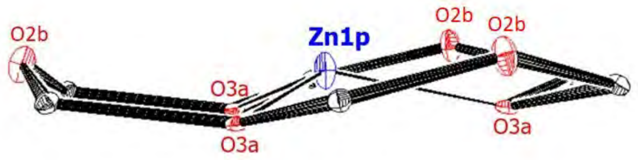
Poster Presentation : **PHYS.P-35**
Physical Chemistry
Event Hall THU 11:00~13:00

Structure Study of Fully Zn^{2+}-exchanged Zeolite Y using Crystallography and NMR

Dae Jun Moon, Woo taik Lim*

Department of Applied Chemistry, Andong National University, Korea

The structures of fully Zn^{2+}-exchanged zeolite Y, $|Zn_{37.5}|[Si_{117}Al_{75}O_{384}]$-FAU, evacuated at 523, 623, 723, 773, and 823 K, were determined at 100 K by single-crystal synchrotron X-ray diffraction in the cubic space group Fd-3m; a = 24.70 to 24.74 Å. At the three highest temperatures, dehydration was complete. In those three, 26 of the 37.5 Zn^{2+} ions per unit cell lie directly in the planes of the two kinds of 6-rings (6Rs, rings containing six oxygen atoms and six tetrahedral atoms (Si or Al)); other Zn^{2+} ions occupied positions on either side of their 6Rs with Zn-O distances 0.1 to 0.3 Å longer. The number of Zn^{2+} ions in these planes closely matches the number of three-Al (3Al) 6Rs calculated by simulated annealing using MAS-NMR data. This indicates that Zn^{2+}, somewhat uniquely because of its ionic size and filled outer shell, is able to lie in the 6R planes of 3Al 6Rs. It lies substantially out of the planes of other 6Rs, predominantly 2Al 6Rs. Thus it is possible to count the number of 3Al 6Rs per unit cell. About 12 of the 32 D6R 6Rs per unit cell, and 14 of the 32 S6Rs, are 3Al 6Rs. This difference is a consequence of the "aluminum avoidance" rule. After vacuum dehydration at 523 and 623 K, water oxygen atoms, ten and six, respectively, were found per unit cell, each bridging between two Zn^{2+} ions in the sodalite cavities; these may be bridging hydroxide ions. The structures (three at each dehydration temperature) were refined using all intensities to final error indices, R_1 for $F_o > 4\sigma(F_o)$, between 0.04 at the lowest dehydration temperature and 0.07 at the highest.


O2b
Zn1p
O2b
O2b
O3a
O3a
O3a


O4
O2a
Zn2p
O4
O4
O2a
O2a

Poster Presentation : **PHYS.P-36**

Physical Chemistry

Event Hall THU 11:00~13:00

A New Diabatization Method for High-Dimensional Coupled Potential Energy Surfaces using Machine Learning

Pinit Ariyageadsakul, Kyoung-Koo Baeck*

Department of Chemistry, Gangneung-Wonju National University, Korea

Diabatic representation of potential energy surface (PES) is an indispensable prerequisite for the nuclear wavepacket propagation studies of reaction dynamics of chemical and biological processes. Diabatization by deep neural network (DDNN) is one of promising methods to construct accurate and smooth diabatic PESs, which allows convenient and semiautomatic diabatization. In this work, we propose a new neural network (NN) approach based on the transfer learning scheme for generating diabatic PESs from adiabatic PESs and a few important diabatic potential energy matrix (DPEM) elements at selected geometries. The MRCI/aug-cc-pVTZ method was employed for evaluating the three lowest adiabatic PESs and DPEM of FHCl, which were used as datasets for machine learning. The diabatic PESs of FHCl are produced by following steps; (1) pretraining NN by adiabatic PESs, (2) transferring the weights from pretrained NN to a new NN and freezing hidden layers, (3) training such NN by DPEM dataset, and (4) fine-tuning the NN obtained from previous step by unfreezing all hidden layers and retraining NN. The adiabatic and diabatic PESs of FHCl given from NN are accurately and smoothly reproduced implying that our diabatization technique is a powerful tool for constructing high dimensional diabatic PESs. The reliability of final DPEM generated by the machine learning is examined by carrying out actual nuclear wavepacket propagation studies.

Poster Presentation : **PHYS.P-37**

Physical Chemistry

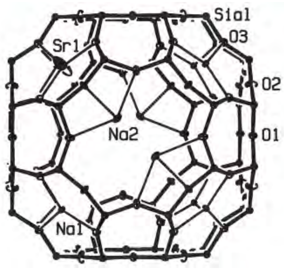
Event Hall THU 11:00~13:00

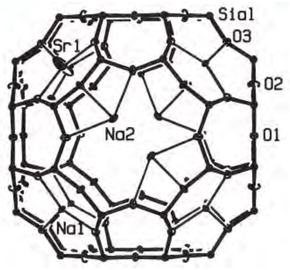
Crystallographic study on the selectivity and distribution of Sr^{2+} ions within zeolite A In the presence of competing Na^{+} ions in aqueous exchange solution

Hu Sik Kim, Hyeon Uk Choo, Ho Yeon Yoo, Woo taik Lim*

Department of Applied Chemistry, Andong National University, Korea

To study the properties of Sr^{2+} exchange into zeolite A with increasing the molar concentration of Na^{+} in given exchange solution, four single crystals of fully dehydrated Sr^{2+}- and Na^{+}- exchanged zeolite A were prepared by the bath method using mixed ion-exchange solutions. The $Sr(NO_3)_2$:$NaNO_3$ molar rations of the ion exchange solution were 1:1(crystal 1), 1:100(crystal 2), 1:250(crystal 3), and 1:500 (crystal 4), respectively, with a total concentration of 0.05 M. The single-crystals were then vacuum dehydration at 623 K and 1 × 10^{-4} Pa for 2 days. Their single-crystal structures were determined by single-crystal synchrotron X-ray diffraction techniques in the cubic space group Pm3-m, at 100(1) K, and were then refined to the final error indices of R_1/wR_2 = 0.047/0.146, 0.048/0.142, 0.036/0.128, and 0.040/0.156 for crystals 1, 2, 3, and 4, respectively. In crystals 1 and 2, the 6 Sr^{2+} ions are found at three different crystallographic sites. In crystal 3, 1 Sr^{2+} and 10 Na^{+} ions are found in large cavity and sodalite unit. In crystal 4, only 12 Na^{+} ions occupy three equipoints. The degree of Sr^{2+} ion-exchange decreased sharply from 100 to 16.7 to 0 % as the initial Na^{+} concentration increase and the Sr^{2+} concentration decrease.





Poster Presentation : **PHYS.P-38**

Physical Chemistry

Event Hall THU 11:00~13:00

Investigation on the factors to influence the sputtering yield of tungsten

Tae Hyun Kwon, Jeong-Woo Nam, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

The sputtering of tungsten samples was performed by bombardment of Ar^+ ions to evaluate the effect of various factors on the sputtering yield. On the basis of the sputtering results for tungsten samples with different surface roughness, we confirmed that the sputtering yield is diminished as the increase in the surface roughness, indicating the inverse relationship between them. When the incident angle of Ar^+ ions increased during the sputtering, the sputtering yield is globally elevated for all tungsten samples regardless of their surface roughness. In addition, we found that the valves of the sputtering yield for tungsten samples under different incident energy of Ar^+ ions are similar within the error of 10 percent.

Poster Presentation : **PHYS.P-39**

Physical Chemistry

Event Hall THU 11:00~13:00

Investigation of the Origin of the Enhanced Photoelectrochemical Performance of Gradient W-Doped $BiVO_4$ Photoanodes

Jungyoon Won, Woon Yong Sohn[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk National University, Korea*

We fabricated gradient W-doped $BiVO_4$ photoanodes to investigate the enhancement of the charge separation efficiency achieved by the electric field in the band bending region. When the concentration of W in the surface of $BiVO_4$ was higher than that in the bulk, the photocurrent density at 1.23 V_{RHE} was improved by about 300 %, compared to that of the bare $BiVO_4$ film, with the cathodic shift of the onset potential. We successfully demonstrated using one of the time-resolved spectroscopic techniques, heterodyne transient grating (HD-TG) technique, and photo-electrochemical impedance spectroscopy (PEIS) that the number of the surface trapped photo-excited holes could increase as increase in the concentration of W in the surface and their recombination could be retarded with aid of the enhanced charge separation.

Poster Presentation : **PHYS.P-40**

Physical Chemistry

Event Hall THU 11:00~13:00

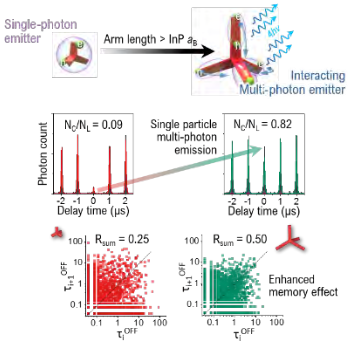
Shape-tuned multi-photon emission in InP nanotetrapods

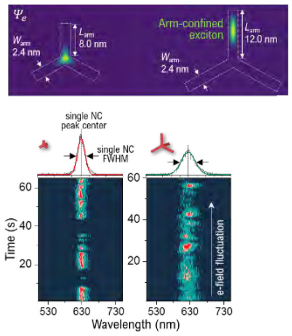
Taehee Kim, Sohee Jeong[1,*], Dongho Kim[*]

Department of Chemistry, Yonsei University, Korea

[1]*Department of Energy Science, Sungkyunkwan University, Korea*

Semiconductors comprise the basis of the modern lifestyle, enabling the everyday technological marvels to take place. Tailoring the property of semiconductor materials has its essence in exciton behavior regulation. In fact, it has long been a primary goal in the field to control exciton behavior in homogeneous semiconductors. In molecular chemistry, the intramolecular exciton-exciton interaction governs the functionality of molecule: in analogy, it is essential to understand how adjacent excitons affect each other in nanocrystals. In this context, we demonstrated a precise control of exciton behavior to understand the exciton-exciton interactions originating from novel single-crystalline tetrapod geometry. Thanks to the unique branched geometry, single crystalline nanotetrapods demonstrated a transition from single to multi-photon emitter upon selective extension of tetrapod arm length. By means of spectroscopic examinations, we revealed that this transition was accompanied by a changeover of exciton confinement orientation from 3D- to 2D-like confinement, which was supported by theoretical calculation results as well. More importantly, exciton-exciton interactions in tetrapodal geometry were realized by various consequences such as enlarged quantum-confined Stark effect, enhanced memory effect, and suppressed Auger recombination. These results highlight the promise of single-crystalline nanotetrapods as a novel platform for tailoring the functionality of nanomaterials. Such geometric tuning of multiple exciton interactions will be a key for future nanomaterial applications.


Single-photon emitter
Arm length > InP a_B
Interacting
Multi-photon emitter
$N_C/N_L = 0.09$
Single particle multi-photon emission
$N_C/N_L = 0.82$
Photon count
Delay time (μs)
-2 -1 0 1 2
$R_{sum} = 0.25$
$R_{sum} = 0.50$
Enhanced memory effect
τ_{i+1}^{OFF}
τ_i^{OFF}
0.1 1 10 100


Ψ_e
W_{arm} 2.4 nm
L_{arm} 8.0 nm
Arm-confined exciton
L_{arm} 12.0 nm
W_{arm} 2.4 nm
single NC peak center
single NC FWHM
Time (s)
20 40 60
e-field fluctuation
530 630 730
Wavelength (nm)

Poster Presentation : **PHYS.P-41**

Physical Chemistry

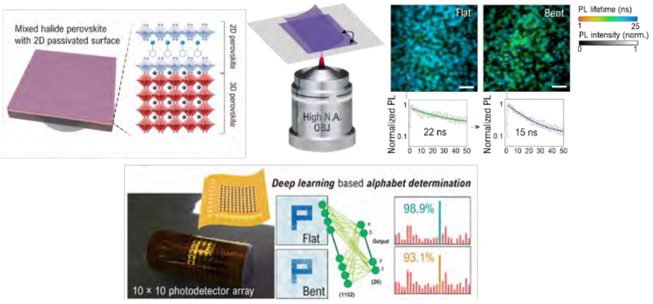
Event Hall THU 11:00~13:00

Engineered Surface Halide Defects in Mixed-halide Perovskite for Flexible Intelligent Photodetectors

Taehee Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Applications of photodetectors are very common in daily life: imaging (i.e. digital cameras), remote control, motion-detecting security, and fire detection. The ultrasensitive photodetection spans in more professional fields as well, such as optical telecommunication, biomedical imaging, and implantable bioelectronics (i.e. artificial eye). When applied for use in photodetectors, the optical properties of semiconductor materials result in varying photoresponse behaviors in terms of responsivity (R), detectivity (D*), response time, and mechanical resistance. Recently, metal halide perovskites have been under spotlight as the most promising photoactive material due to their outstanding optical properties. Their long charge carrier diffusion length and high defect tolerance suggest perovskite materials a great advantage for various optoelectronic applications. In particular, Perovskites with mixed chemical compositions are advantageous to expand the material's applicability, since their optical properties are easily tuned by varying the precursor ratio. However, their mixed chemical compositions often accompany photoelectric instability issues such as photoinduced halide segregation. Herein, we post-treated the perovskite surface in an attempt to reduce halide segregation and succeeded in demonstrating the flexible perovskite photodetectors with an excellent image-sensing performance. Successful demonstration of intelligent and flexible perovskite photodetector will pave the way in furthering the development of the next generation optoelectronics.



Poster Presentation : **PHYS.P-42**

Physical Chemistry

Event Hall THU 11:00~13:00

Structural Dynamics of $C_2F_4I_2$ in Cyclohexane Studied via Time-Resolved X-ray Liquidography

Jain Gu, Hosung Ki[1], Seunghwan Eom, Yunbeom Lee[1], Jeongho Kim[2], Hyotcherl Ihee[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1] *Center for Advanced Reaction Dynamics, Institute for Basic Science, Korea*
[2] *Department of Chemistry, Inha University, Korea*

The halogen elimination of 1,2-diiodoethane ($C_2H_4I_2$) and 1,2-diiodotetrafluoroethane ($C_2F_4I_2$) serves as a model reaction for investigating the influence of fluorination on reaction dynamics and solute–solvent interactions in solution-phase reactions. While the kinetics and reaction pathways of the halogen elimination reaction of $C_2H_4I_2$ were reported to vary substantially depending on the solvent, the solvent effects on the photodissociation of $C_2F_4I_2$ remain to be explored, as its reaction dynamics have only been studied in methanol. Here, to investigate the solvent dependence, we conducted a time-resolved X-ray liquidography (TRXL) experiment on $C_2F_4I_2$ in cyclohexane. The data revealed that (i) the solvent dependence of the photoreaction of $C_2F_4I_2$ is not as strong as that observed for $C_2H_4I_2$, and (ii) the nongeminate recombination leading to the formation of I_2 is slower in cyclohexane than in methanol. We also show that the molecular structures of the relevant species determined from the structural analysis of TRXL data provide an excellent benchmark for DFT calculations, especially for investigating the relevance of exchange-correlation functionals used for the structural optimization of haloalkanes. This study demonstrates that TRXL is a powerful technique to study solvent dependence in the solution phase.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-43**

Physical Chemistry

Event Hall THU 11:00~13:00

Single-molecule observation of spiropyran dimerization

Dokyung Jeong, Doory Kim*

Department of Chemistry, Hanyang University, Korea

Spiropyran is a photochromic compound that is reversibly converted into a colored merocyanine. This coloration change can be induced by various stimulants, such as UV light, metal ions, thermal energy, and mechanical stress. Although the individual observation of various structural change mechanisms of spiropyran has been generally masked in the ensemble averages of previous bulk measurements, the recent study using spectrally resolved stochastic optical reconstruction microscopy (SR-STORM) demonstrated the identification of the two isomers of merocyanine molecule depending on the solvent polarity by measuring their single-molecule spectra in real time. Related to this previous study, we here observed the solvent-dependent spiropyran dimerization reactions at the single-molecule level for the first time. We observed two distinct dimerization reactions depending on the solvents; radical-mediated dimerization and dimerization through π- π stacking interaction. We demonstrate that SR-STORM can be a powerful technique to define various reaction mechanisms of photochromatic compounds at the single-molecule level.

Poster Presentation : **PHYS.P-44**

Physical Chemistry

Event Hall THU 11:00~13:00

Development of ultralow-laser-power STORM nanoscopy

Uidon Jeong, Doory Kim[1,*], Dokyung Jeong[2]

Department of Chemistry, Hanyang University, Korea, Hanyang University, Korea

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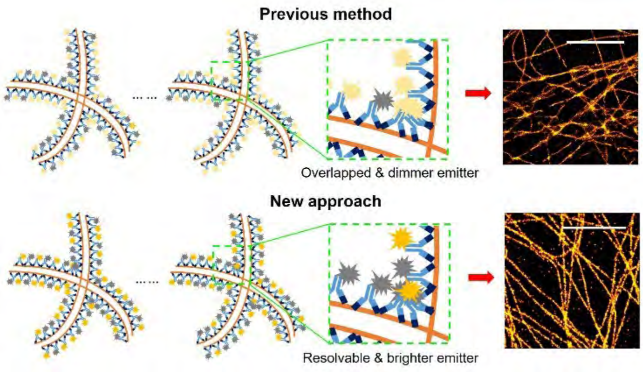
[2]*Department of chemistry, Hanyang University, Korea*

The rise of super-resolution fluorescence microscopy over the past decade has drastically improved the resolution of light microscopy to ~10 nm. Among these methods, stochastic optical reconstruction microscopy (STORM) can be used to achieve sub-diffraction-limit resolution by sequentially imaging and localizing individual photoswitchable fluorophores. It is known that the switching rate of photoswitchable fluorophores depends on the laser power—a high laser power being required for the enhancement of imaging resolution. However, such high laser power usually results in photobleaching and high photo-toxicity effects, making it harmful to power-sensitive specimens, including biological samples. In this study, we attempted to overcome this problem by improving the STORM resolution at a lower laser power. Through the quantitative analysis of the photoswitching behavior of single fluorophores under different laser power conditions, we developed a new approach to achieve super-resolution fluorescence images at a laser power 10 times lower than had previously been reported. This approach is expected to play an increasingly significant role in super-resolution imaging of power-sensitive samples, such as live cells.



Poster Presentation : **PHYS.P-45**

Physical Chemistry

Event Hall THU 11:00~13:00

Benzene and Ammonia removal over activated carbon under visible light

Miyeon Jeong, Shufang Zhao, HuiCheol Choe, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

Benzene and ammonia removal efficiency over activated carbon (AC) at various relative humidity (RH) levels (0%, 30%, 60%) were studied under dark and visible-light conditions. The benzene removal efficiency decreased with increasing humidity under either dark or light, the effect that can be attributed to competitive adsorption between benzene and water molecules on the AC surface. Moreover, the benzene removal rate enhanced after light exposure, which suggested that the electron-hole pair formed by electron transition generates active oxygen through interaction with oxygen and water molecules, thereby improving the adsorption capacity of benzene on the AC surface and partially oxidizing it. While the ammonia removal efficiency was changed with increased humidity, the ammonia removal rates and breakthrough time increased as the humidity increased to 30% RH, whereas reduced under higher humidity (60% RH). Furthermore, the breakthrough time was reduced by ammonia desorption with light irradiation, but the removal rate was increased as the hydroxyl radical generated by the interaction of holes and water molecules on the AC surface oxidized ammonia. We highlight the different structural information of the AC surface, depending on the reactions and conditions.

Poster Presentation : **PHYS.P-46**
Physical Chemistry
Event Hall THU 11:00~13:00

Molecular Modeling of PEDOT:PSS Treated with Hard-Cation-Soft-Anion Ionic Liquids

Changwon Choi, Minji Kim[1], Minwoo Han[2], Haemin Choi[2], Byoung Hoon Lee[1,*], Seoung Ho Lee[3,*], Yves Lansac[4,*], Yun Hee Jang[5,*]

Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Chemical Engineering and Materials Science, Ewha Womans University, Korea*
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[4]*GREMAN, Department of Physics, Korea*
[5]*Energy Science and Engineering, DGIST, Korea*

Poly(3,4-ethylenedioxythiophene):poly(stryrenesulfonate) (PEDOT:PSS), a polymer electrolyte composed of positive-charged PEDOT and negative-charged PSS, has received great attention as a flexible, lightweight, transparent, and low-cost organic semiconductor and electrochemical transistor, which can be used for various applications. The long, hydrophilic, and insulating PSS chains contribute to the water solubility and stability of PEDOT:PSS by encapsulating the short, hydrophobic, and conducting PEDOT chains, but they are also responsible for the poor electric conductivity and mobility of pristine PEDOT:PSS by interfering with network formation of PEDOT-rich conducting domains. Dramatic improvement of PEDOT:PSS conductivity has been achieved by ionic liquid (IL). Various observations, both experimental and computational, have indicated a mechanism in which an ion exchange between PEDOT:PSS and IL triggers PEDOT:PSS separation, PEDOT self-assembly, and formation of PEDOT-rich domains decorated by IL anions. This mechanism naturally leads to a molecular design principle that ILs or ionic salts with hydrophilic (hard) cations and hydrophobic (soft) anions would favor such processes, as demonstrated by a recent experiment. Moreover, this experiment also showed a improvement of the elasticity and stretchability of PEDOT:PSS treated with such hard-cation-soft-anion ILs. Therefore, in this work, we build a molecular model for a thin film of IL-treated PEDOT:PSS deposited from the aqueous solution and carry out a multiscale molecular modeling combining quantum-mechanical density functional theory calculations

and classical molecular dynamics simulations to understand the IL dependence of such improvements in electric conductivity and elastic modulus at the molecular level.

Poster Presentation : **PHYS.P-47**

Physical Chemistry

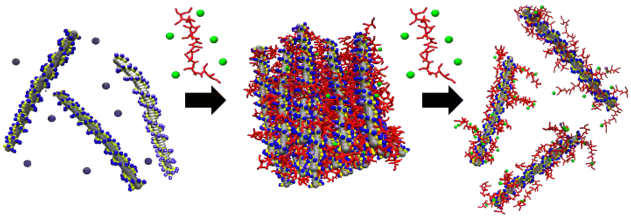
Event Hall THU 11:00~13:00

Protamine-Controlled Reversible DNA Packaging. A Molecular Glue.

Yves Lansac[*], **Yun Hee Jang**[1,*]

GREMAN, Department of Physics, University of Tours, France
[1]*Department of Energy Science and Engineering, DGIST, Korea*

While DNA is one of the longest and stiffest molecules in nature and is negatively charged, they are strongly condensed in a tiny space of cell nuclei. DNA undergo precise cycles of even stronger condensation and decondensation during cell division or in sperm cells. Packaging paternal genome into tiny sperm nuclei during spermatogenesis requires 10^6-fold compaction of DNA, corresponding to a 10-20 times higher compaction than in somatic cells. Understanding molecular principles underlying such fascinating dynamic processes will not only bring us a step closer to the origin of life but also have applications in various fields of medicine, materials, and energy. While protamine, a small arginine-rich basic protein, is known to participate in such a high level of compaction, the precise mechanism at play is still unclear. Herein, effective pair potential calculation and large-scale molecular dynamics simulation using a simple idealized model incorporating solely electrostatic and steric interactions clearly demonstrate a reversible control on DNA condensate formation by varying the protamine-to-DNA ratio. Microscopic states and condensate structures occurring in semi-dilute solutions of short DNA fragments are in good agreement with experimental phase diagram and cryoTEM observations. This microscopic mechanism of reversible protamination modulation can improve a mechanistic understanding of early and intermediate stages of spermatogenesis where an interplay between condensation and liquid-liquid phase separation triggered by protamine expression and post-translational regulation might occur. Recent mRNA vaccines against virus infections and cancers using protamine as packaging-depackaging agent can be tuned for improved efficiency with protamination control.



Poster Presentation : **PHYS.P-48**

Physical Chemistry

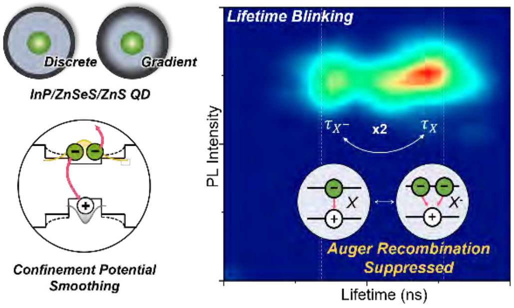
Event Hall THU 11:00~13:00

Lifetime Blinking in InP/$ZnSe_xS_{1-x}$/ZnS Quantum Dots

Yu Jin Lee, Taehee Kim, Jumi Park, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

In this study, we find that 'lifetime blinking' can be observed in environment-friendly interface alloyed InP/$ZnSe_xS_{1-x}$/ZnS quantum dots (QDs) with optimal composition. Auger recombination is known to be one of the major drawback factors for self-emitting quantum dot light-emitting diode (QLED) display efficiently. We scrutinize the effect of various ZnSeS midshell compositions on QD performance and find the relationship between shell structure/composition and QD performance. Negative trion Auger recombination dynamics are studied through ensemble and single-dot analysis. Interface alloying successfully reduce lattice difference and smoothen confinement potential, and therefore, substantially suppress unwanted Auger recombination. Nonradiative Auger rates are found to decrease from 0.41 ns^{-1} to 0.022 ns^{-1} with the introduction of a smooth shell interface. Properties regarding photoluminescence (PL) peak width, including spectral diffusion and single-dot PL peak width, are also improved with the introduction of gradient shells due to reduced lattice mismatch between shells and increased charge trapping energy barrier. Yet, these performance improvements are found to be composition-dependent, requiring ZnSe rich midshell to prevent lattice strain in the interface of the core and the shell from arising.



Poster Presentation : **PHYS.P-49**

Physical Chemistry

Event Hall THU 11:00~13:00

TDDFT and High-level Ab Initio Study of Excited States of Thiomaleimide

Dakyeung Oh, Seongjae Lee, Joonghan Kim*

Department of Chemistry, The Catholic University of Korea, Korea

We performed time-dependent density functional theory (TDDFT) calculations of the excited states of thiomaleimide. The excitation characters of S_1 and S_2 states are $\pi\pi^*$ and $n\pi^*$, respectively. The order of excited states differs from that of maleimide. We also performed high-level ab initio methods such as equation-of-motion coupled-cluster singles and doubles (EOM-CCSD) and multi-state complete active space second-order perturbation theory (MS-CASPT2) to compare the results with those of TDDFT. The results of EOM-CCSD and MS-CASPT2 are the same as those of TDDFT. We discuss the substituent effect on the order of excited states.

Poster Presentation : **PHYS.P-50**

Physical Chemistry

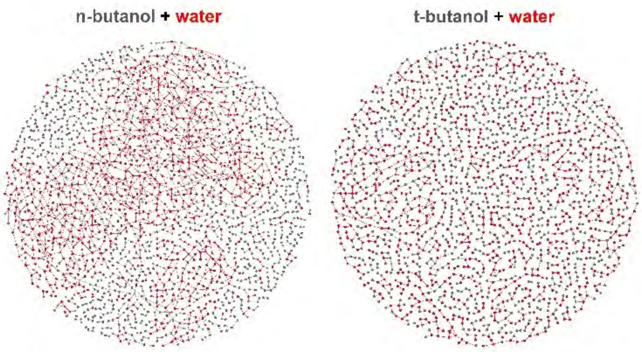
Event Hall THU 11:00~13:00

Graph theoretical analysis on alcohol aggregation and water H-bond network in alcohol-water mixture

Seungeui Choi, Jun-Ho Choi[*]

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Research on understanding aqueous solutions from a molecular level perspective has received attention for a long time. In recent years, many studies have been carried out to investigate the water hydrogen-bond network and the aggregation of solute in aqueous solution through molecular dynamics (MD) simulations. Among various solutes such as ion, osmolyte, and protein, alcohol aggregation behavior in aqueous solution is a subject of considerable attention due to its self-association and diverse solubility depending on the type. Several factors such as temperature and polarity of alcohol have a significant impact on the phase behavior of this alcohol-water mixture. In this work, it is shown how the alcohol chain length, molecular shape of alcohol isomers, and temperature affect the aggregation behavior of alcohol and water H-bond network in alcohol solutions. By employing MD simulation and graph theoretical analysis, the network properties of alcohol and water H-bond aggregates were examined quantitatively and the distinct aggregation pathway was proposed to explain the phase behavior of binary liquids.



water-incompatible network ***water-compatible network***

Poster Presentation : **PHYS.P-51**

Physical Chemistry

Event Hall THU 11:00~13:00

GB agent capture using anionic metal cluster

ChangJun Park, Sang Hak Lee*

Department of Chemistry, Pusan National University, Korea

Chemical weapons which can make mass destruction are extremely lethal to humans. Since most chemical weapons are gaseous and aerosolized agents, they float around in the atmosphere and so it is difficult to remove the reagent immediately. Therefore, a critical step is capturing the reagent in the gas phase to convert it to a safe chemical for us. It is well-known that highly toxic chemical weapons have halogen elements. Thus, we thought that the reagents can be captured using anionic metal clusters and be induced chemical reactions. In this study, we carried out theoretical calculations for the reactivity of various metal clusters, such as coinage metals, with Sarin (GB in military design) using density functional theory with various functionals. We found that specific anionic metal clusters strongly interacted with the GB agent in the gas phase. We also learned that more anionic charges in metal clusters induce much stronger interaction with the GB agent.

Poster Presentation : **PHYS.P-52**

Physical Chemistry

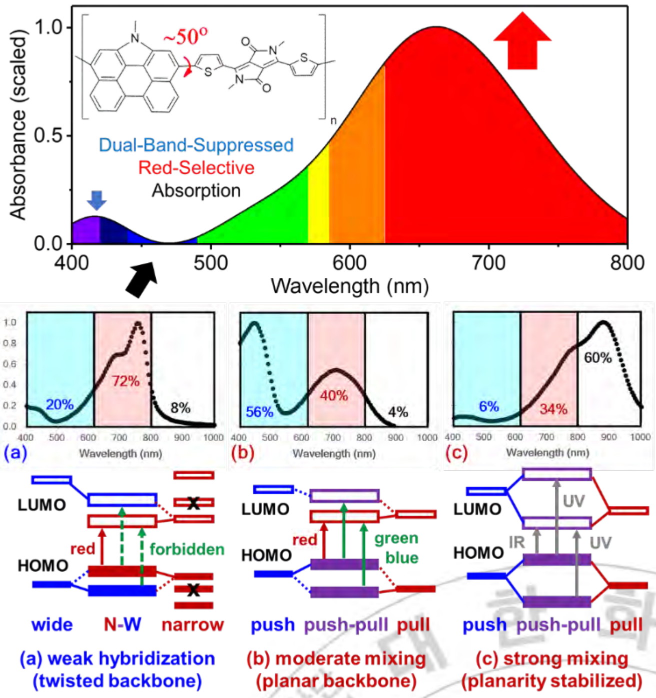
Event Hall THU 11:00~13:00

Copolymer Design Improving Red-Color-Selective Strong Absorption

Changwon Choi, Yun Hee Jang*

Department of Energy Science and Engineering, DGIST, Korea

Organic full-color image sensors require color-selective organic-photodiode components. The most challenging components are those for red-selective absorption (625-800 nm), often accompanied by higher-energy absorption in the green and blue regions (400-625 nm). Push-pull polymers with suppressed high-energy bands have been designed and synthesized, but the low-energy bands of these polymers are extended to IR region (>800 nm). This is useful for photovoltaics but not for sensitive red-color detection. Herein we define the red selectivity (RS, %) as the ratio of absorption in the red region (the area under the absorption spectrum between 625 and 800 nm) to the total absorption in the visible and near-IR regions (the area under the absorption spectrum between 400 and 1000 nm). We also propose an RS-enhancing copolymer design rule, (1) HOMO and LUMO localized in the narrow-band-gap unit and HOMO-1 and LUMO+1 localized in the other wide-band-gap unit and (2) hybridization between the two units minimized by introducing a twist in the backbone). Copolymers of thiophene-flanked diketopyrrolopyrrole (T-DPP-T) narrow units linked to benzene, naphthalane, or phenanthrocarbazole wide units indeed exhibit high RS values (75%).



Absorbance (scaled)
1.0
0.5
0.0
~50°
n
Dual-Band-Suppressed
Red-Selective
Absorption
400
500
600
700
800
Wavelength (nm)
20%
72%
8%
56%
40%
4%
6%
34%
60%
Wavelength (nm)
(a)
(b)
(c)
LUMO
HOMO
red
forbidden
wide
N-W
narrow
green
blue
push
push-pull
pull
IR
UV
(a) weak hybridization
(twisted backbone)
(b) moderate mixing
(planar backbone)
(c) strong mixing
(planarity stabilized)

Poster Presentation : **PHYS.P-53**

Physical Chemistry

Event Hall THU 11:00~13:00

Diffusiophoretic Flows in Microchannels Simulated by a Coupled Method of Molecular Dynamics and Multiparticle Collision Dynamics

Jaeyoung Gil, Shang Yik Reigh[1], YounJoon Jung*

Department of Chemistry, Seoul National University, Korea
[1]*The Research Institute of Basic Sciences, Seoul National University, Korea*

In experiments one often observes fluid flows in the presence of concentration or temperature gradients on fixed surfaces, for example in glasses or microchannels. These phoretic flows may induce the motions of passive particles and as well play important roles in the dynamics of phoretic particles and thereby their collective behaviors. Here we consider diffusiophoretic flows which arise from the concentration gradients of neutral particles and develop a new particle-based simulation method using a coupled method of molecular dynamics and multiparticle collision dynamics. Molecular interactions adopted in simulations produce proper no-slip boundary conditions and under an external force Poiseuille flows are created. For a diffusiophoretic flow, the steady state concentration gradients for two chemical species are built along the microchannel. Introducing different interaction potentials between the chemical species and the surfaces, we observed the steady diffusiophoretic fluid flows are indeed created along the channel.

Poster Presentation : **PHYS.P-54**

Physical Chemistry

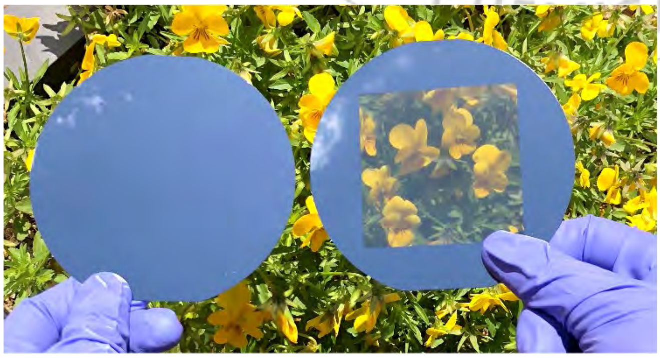
Event Hall THU 11:00~13:00

Neutral-color Semi-transparent Crystalline Silicon Solar Cells

Kangmin Lee, Kwanyong Seo*

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

In this presentation, we show a novel approach to develop neutral-color transparent c-Si solar cells. First of all, we have developed a neutral-color transparent c-Si substrate using a 200-μm thick c-Si wafer, which is known to be opaque. In this semi-transparent substrate, a light transmitting area was designed to enable all incident visible light to be transmitted through the substrate, in order to achieve a colorless substrate. A light absorption area was also designed on the substrate to efficiently absorb incident light of the spectral range between 300 nm and 1100 nm. The transmittance of the transparent c-Si substrate was systematically tuned from 20% to 50 % under the full solar spectrum. The semi-transparent solar cells fabricated with the substrate exhibit a power conversion efficiency of up to 12.2%, with J_{sc} = 29.2 mA·cm^{-2}; V_{oc} = 588 mV; and FF = 71.1% with a transmittance of 20 %. Hence, our novel c-Si semi-transparent solar cells presents a unique opportunity to develop next-generation neutral-color semi-transparent solar cells which would satisfy high efficiency as well as high stability.



Poster Presentation : **PHYS.P-55**

Physical Chemistry

Event Hall THU 11:00~13:00

Effect of the enhanced solvent-solute interaction in the deeply supercooled regime on the structure of triiodide ion

Kyeongmin Nam, Seonju You, Kyung Hwan Kim*

Department of Chemistry, Pohang University of Science and Technology, Korea

Solvent-solute interaction is one of the key factors to comprehend various mechanisms and properties of the molecules. One such interaction is the hydrogen bonding interaction, which is common in aqueous solutions. Recent studies on I3- revealed that the hydrogen-bonding solvents make the solute have an asymmetric and bent structure due to the strong solvent-solute interaction. Since it is well known that the hydrogen bonding network gets stronger at supercooled temperatures, we have studied I3- in supercooled solution to understand the effect of the enhanced solvent-solute interaction.[1] K. H. Kim et al., Phys. Rev. Lett. 110, 165505 (2013)[2] K. H. Kim et al., Science 358, 1589-1593 (2017)

Poster Presentation : **PHYS.P-56**

Physical Chemistry

Event Hall THU 11:00~13:00

Revealing the Reaction Mechanism of Nickel-Catalyzed Cross-Coupling Reaction by Using Time-Resolved X-ray Absorption Spectroscopy

Yeseul Han, Kyung Hwan Kim[1,*]

Chemistry, Pohang University of Science and Technology, Korea

[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Carbon-oxygen cross coupling reaction with nickel catalyst is one of the most intense research subjects. They are uncommon since the essential step for the reaction (the reductive elimination of the Ni^{II} intermediate) is known to be unfavorable. Introducing photo-excitation can be a solution to the difficulty, but its mechanism is ambiguous. With Ir photocatalyst, the excited photocatalyst could activate the Ni^{II} intermediate by excitation or a redox reaction (1-2). Also, the direct excitation mechanism has been proposed in which excited Ni causes the reaction itself through aryl homolysis (3). Even though these mechanisms have been suggested and under fierce debate, there is no direct experimental evidence to point which mechanism is correct since it is hard to distinguish the Ir photocatalyst and the Ni intermediates in the UV-visible region (4). In this work, we predict the XANES spectrum of the Ni intermediate using theoretical calculation and demonstrate the feasibility of the XANES experiment distinguishing the Ni intermediates having different oxidation states. With extremely intense X-ray sources, such as an X-ray free electron laser, the TR-XANES technique will be the advantageous approach to explain the reaction mechanism of the Ni catalyst. Reference [1] E. R. Welin et al., Science 2017, 355, 380-385 [2] R. Sun, Y. Qin, D. G. Nocera, Angew. Chem. Int. Ed. 2020, 59, 9527-9533 [3] S. I. Ting et al., J. Am. Chem. Soc. 2020, 142, 5800-5810 [4] L. Tian et al., J. Am. Chem. Soc. 2020, 142, 4555-4559

Poster Presentation : **PHYS.P-57**

Physical Chemistry

Event Hall THU 11:00~13:00

Ring-opening reaction of the five-membered cyclic ether on Ge(100)

Jeong-Woo Nam, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

We investigated the adsorption structures and mechanisms of tetrahydrofuran, a five-membered cyclic ether, on a Ge(100) surface using the combination of high-resolution photoemission spectroscopy (HRPES) and density functional theory (DFT) calculations. In O 1s core-level spectrum, We observed two distinct peaks at 531.6 and 533.5 eV, which are attributed to the adsorption configurations of Ge-$(CH_2)_4$-O-Ge structure through the ring-opening reaction and C_4H_8O-Ge structure via O dative bonding, respectively. On the basis of DFT results with the optimized adsorption energies for their corresponding adsorption structures, we confirmed that the two adsorption geometries are formed in the system of tetrahydrofuran on the Ge(100) surface.

Poster Presentation : **PHYS.P-58**

Physical Chemistry

Event Hall THU 11:00~13:00

Photoionization dynamics and cationic structures of cyclopentanone and 2-cyclopentenone by high-resolution VUV-MATI mass spectroscopy

Yu Ran Lee, Chan Ho Kwon[1,*]

Forensic Chemistry Division, National Forensic Service, Korea

[1]*Department of Chemistry, Kangwon National University, Korea*

Cyclopentanone (CP) and 2-cyclopentenone (2CP) have received much attention because of their versatile functionality in the synthesis of materials for biofuels. In particular, since two molecules exhibit flexible structures with a ring puckering or twisting motion, checking their related conformational structures is prerequisite, resulting in the development of associated potential energy surfaces. We have investigated the conformational structures and the photoionization dynamics of the corresponding conformers in CP and 2CP utilizing the high-resolution vacuum ultraviolet mass-analyzed threshold ionization (HR VUV-MATI) mass spectroscopy. Notably, the adiabatic ionization energy of 2CP (9.3477 ± 0.0004 eV) is higher than that of CP (9.2704 ± 0.0002 eV). It implies that although the highest occupied molecular orbital (HOMO) of each corresponded conformer, which mainly consists of nonbonding orbitals on the oxygen atom in the carbonyl group interacting with the □ orbitals in the ring is similar, the HOMO of 2CP should be additionally stabilized due to a plane geometry of the C=C and C=O bonds. Furthermore, it was found that the low photon energy of ~ 9.7 eV above the ionization onset of the twisted conformer in only CP could lead to ring opening dissociation. Meanwhile, the cationic geometries of CP and 2CP have the C1 symmetry lowered with respect to the symmetry of each neutral geometry, which could be realized from the fact that such geometrical changes are mainly attributed to the electron removal from the HOMO.

Poster Presentation : **PHYS.P-59**

Physical Chemistry

Event Hall THU 11:00~13:00

Molecular dynamics simulation study of the effect of cholesterol on doxorubicin permeation through the membrane of drug-resistant cancer cells

Hyonseok Hwang*, Namho Kim[1]

Department of Chemistry, Kangwon National University, Korea

[1]*Department of biochemistry, Kangwon National University, Korea*

We conducted all-atom molecular dynamics (AA MD) simulations to elucidate the effect of cholesterol lipids on doxorubicin (DOX) permeation through drug—resistant cancer cell membrane. We constructed two simplified model membranes: a 1-palmitoyl-2-oleoyl-glycero-3-phosphocholine (POPC) symmetric bilayer modeling a normal cell membrane and a complex bilayer composed of 50% POPC and 50% cholesterol (CHOL) bilayer modeling a drug-resistant cancer membrane and then observed the behavior of a DOX molecule on those models. Free energy profiles of DOX as a function of distance between DOX and the bilayer center show a higher energy barrier in the complex model. In addition, the orientation of DOX inside the bilayers significantly affects the free energy profiles. In pure model, DOX has unfavorable orientation to downward as the orientation makes it difficult to interact with lipid head group or water. Meanwhile, DOX favors to have either up or downward orientation in complex model due to the strong membrane packaging effect of CHOL which makes it hard for DOX to be placed parallel to membrane axis. While a huge energy barrier is observed at $z = 20$ Å when DOX is oriented downward in complex model, it is not in pure model. It turned out that the presence of CHOL in the complex model leads to DOX having more hydrogen bonds with nearby lipids. Finally, when DOX is located in membrane center, several water molecules permeate and form hydrogen bonds in pure model, but it is not observed in complex model. Taken these together, the most important factors affecting the free energy variation for DOX membrane permeation are hydration and orientation. Because the presence of CHOL significantly disrupts those factors, DOX resistant cancer cells could utilize this as a defense strategy.

Poster Presentation : **PHYS.P-60**

Physical Chemistry

Event Hall THU 11:00~13:00

Mechanism Study of Selective Photocatalytic Conversion of HMF to FDCA using Co3+ ion Doped ZnO Nanoparticles

Vy Pham, Hangil Lee*

Department of Chemistry, Sookmyung Women's University, Korea

We conducted the catalytic redox reaction of 5-hydroxymethylfurfural (HMF) molecules, which has been widely used in recent studies on the redox reaction of biomass molecules. It is very important to study the mechanism of oxidation reaction using photocatalyst of HMF, which is used as a precursor of alternative substances in petrochemicals. It is also important to identify the selective products in each oxidation reaction. To confirm the mechanism of the selective redox reaction, the photocatalytic properties change was confirmed using Co ions with different charge states doped into ZnO NPs. Here, we demonstrate that the number of oxygen vacancies generated by Co ion-doping (Co3+ or Co2+) determines the photocatalytic degradation (PCD) activity for organic pollutants, depending on the charge mismatch. As a result, we found that Co3+ ion doping leads to a significant enhancement of the PCD activity of the ZnO NPs and exhibits selectively oxidation reaction with good yield (~97 %) by changing HMF to FDCA via 5-hydroxymethyl-2-furan carboxylic acid (HMFCA).

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-61**

Physical Chemistry

Event Hall THU 11:00~13:00

Identification of individual conformers in *trans*-2-pentenal by the IR resonant VUV-MATI mass spectroscopy

Sung Man Park, Chan Ho Kwon[*]

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

The *trans*-2-pentenal (*trans*-2PA) has two main conformations, the s-*trans* and s-*cis* in equilibrium, which can be interconverted by rotating along the C-C bond between C=O and C=C double bonds. In addition, it is expected that the non-planar conformation such as *gauche* arises from the terminal methyl group. In recent, we have developed the conformer-specific vibrational spectroscopic techniques capable of measuring the identifiable vibrational spectra of the individual conformers in the neutral (S_0) and cationic (D_0) states. We investigated the conformations of *trans*-2PA in the S_0 and D_0 states using IR resonant HR VUV-MATI mass spectroscopy. The conformer-specific IR spectra in the C-H region of *trans*-2PA in the S_0 state could be measured by IR dip VUV-MATI spectroscopy and thereafter the cationic vibrational spectra of individual conformers could be measured by IR hole-burn VUV-MATI spectroscopy based on the measured conformer-specific IR spectra in the S_0 state. As a results, we observed the origin bands corresponded to two stable conformations of *cis* and *gauche* in s-*trans* conformation, s-*trans-cis* and s-*trans-gauche* conformers. Accordingly, the adiabatic ionization energies of two stable conformers could be determined based on their origin bands. Variation experiments of molecular beam conditions revealed that the s-*trans-cis* conformer is more stable than the s-*trans-gauche* conformer. Finally, the relative populations of s-*trans-cis* and s-*trans-gauche* conformers in *trans*-2PA could be determined using the IR dip intensities, the Franck-Condon factors, and calculated IR absorption probabilities for two conformers.

Poster Presentation : **PHYS.P-62**

Physical Chemistry

Event Hall THU 11:00~13:00

Enhanced PEC Efficiency by Heterojuction Photocatalyst for Solar Water Splitting

Myung jong Kang

Department of Chemistry, Gangneung-Wonju National University, Korea

Fabricating heterojuction structure is one of the noticeable strategies on enhancing PEC efficiency of photoelectrode. In this aspect, $BiVO_4$ (BVO) is widely studied oxide for PEC catalyst because of its high charge extraction yield and high catalytic properties derived from surface oxygen vacancies. However, poor electron-hole separation of BVO leads poor reaction kinetics during PEC reaction in solar water splitting reaction. Here, we studied on fabricating heterojuction structure of BVO photoanode with thin carbon layer for increasing electron-hole separation and transport efficiency. By constructing hetrojuction photoelectrode with BVO and thin carbon layer, noticeable photocatalytic efficiency enhanced was observed in solar water splitting reaction. The reasons for enhanced PEC efficiency of BVO-carbon heterojuction photoanode was revealed to efficiency charge transfer during PEC reaction.

Poster Presentation : **PHYS.P-63**

Physical Chemistry

Event Hall THU 11:00~13:00

Melamine-formaldehyde resin and Urea Derived Carbon Nitride as an Pollution Removal Photocatalyst

Jae Hyun Park, Serin Jung, Myung Jong Kang[1,*]

Gangneung-Wonju National University, Korea

[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Melamine-formaldehyde resin (MF), a sort of thermoset plastic, is regarded as major concern on plastic waste contamination on the earth due to its difficulty on natural degradation. Herein, we studied on possibility of recycling waste MF as a noticeable precursors on synthesizing photocatalyst for water purification. The urea mixed with MF used as precursor of g-C_3N_4 photocatalysts by thermal treatment process, with varying MF amount into urea (FX, X= MF amount). The structural and optical properties of synthesized MF added g-C_3N_4 was measured by IR, UV-vis and TEM analyses. Photocatalytic efficiency of synthesized catalysts was evaluated by degrading methyl orange (MO) solution, as an model compound of organic pollutant in water. The MF added g-C_3N_4 showed enhanced photocatalytic efficiency by comparing pure g-C_3N_4. Thus, this study suggest the noticeable possibility on recycling waste melamine resin as an additive during synthesizing photocatalyst for water purification.

Poster Presentation : **PHYS.P-64**

Physical Chemistry

Event Hall THU 11:00~13:00

Additive Effect on Solvation Structure of Organic Carbonate Electrolytes for Lithium-Ion Battery

Jiyeon Yang, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

In the development of lithium-ion batterys(LIBs), it is important to study electrolytes because the electrolyte is a charge carrier which is essential to the battery reaction. There are various types of electrolytes, but among them, the organic carbonate electrolyte is most often used because of its high ion conductivity. But there is a limit to poor electrochemical stability problems of them. To solve this problem, there have been many reports about electrolyte additives that significantly improve the cycle life of LIBs. For better battery performance, it is important to understand the solvation nature of lithium-ion not only in the organic carbonate electrolytes but also with additives. We represent the effect of additives on solvation structure especially by using vibrational spectroscopy. Vibrational spectroscopy tools give us information about the in situ or in operando observation of nature around lithium ions and help to determine coordination number.

Poster Presentation : **PHYS.P-65**

Physical Chemistry

Event Hall THU 11:00~13:00

Direct observation of ligand dissociation reaction of $Os_3(CO)_{12}$ using time-resolved X-ray liquidography

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$Os_3(CO)_{12}$ is one of the representative photocatalysts suggested in classical inorganic chemistry. $Os_3(CO)_{12}$ has the advantage of being stable compared to $Fe_3(CO)_{12}$, which is a similar type of photocatalyst. Despite this representativeness and stability, the structural dynamics of $Os_3(CO)_{12}$ have not yet been elucidated. On the other hand, it is known that $Os_3(CO)_{12}$ is exposed to a 267 nm laser pulse and the CO ligand dissociates. Identification of the reaction intermediates in which these ligands are separated will help to understand the mechanism of photocatalysis. Therefore, we used time-resolved x-ray liquidography, a structure-sensitive tool, to observe the ligand dissociation reaction of $Os_3(CO)_{12}$ in real-time. This study will provide information on the structural dynamics of reaction intermediates that occur under 267 nm laser exposure.

Poster Presentation : **PHYS.P-66**

Physical Chemistry

Event Hall THU 11:00~13:00

Energetics of Anionic Surfactant Transfer from a Micelle to Ceramide and Phospholipid Bilayers: A Molecular Dynamics Simulation Approach

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We investigated the characteristic behavior of a surfactant micelle on model ceramide and DMPC lipid bilayers using molecular dynamics (MD) simulation. Sodium lauryl 2-ether sulfate (SLE2S), which is an anionic detergent and surfactant found in many personal care products, was selected as the main component of the micelle. Our previous constant-force steered molecular dynamics (cf-sMD) revealed that a single SLE2S micelle has different shapes on the C24 ceramide (d18:1/24:0) or the 1,2-dimyristoyl-sn-glycero-3-phosphorylcholine (DMPC) bilayer; an upper hemispherical form in the ceramide bilayer and and a spherical shape in the DMPC bilayer.[1] In this study, the two dimensional potential of mean force (2D-PMF) calculations show the distinct energy landscapes in the SLE2S surfactant transfer from a micelle to the two different types of bilayers. The transfer of SLE2S to the C24 ceramide bilayer from a micelle is energetically more favorable than to the DMPC bilayer. The PMF profiles at 313.15 K and 350.15 K, which were calculated to investigate the temperature dependence of SLE2S migration from a micelle into the two types of bilayers, indicate that the energy barriers are reduced in the transfer into the C24 ceramide bilayer as the temperature increases. In the case of the DMPC bilayer, however, the substantial temperature dependence was not observed in the PMF profiles.1. Y. Song, J. H. Lee, I. Jung, B. Seo, and H. Hwang, “Molecular Dynamics Simulations of Micelle Properties and Behaviors of Sodium Lauryl Ether Sulfate Penetrating Ceramide and Phospholipid bilayers”, J. Phys. Chem. B 124, 5951 (2020).

Poster Presentation : **PHYS.P-67**

Physical Chemistry

Event Hall THU 11:00~13:00

Charge-delocalized state and coherent vibrational dynamics in PBI H-aggregates

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Herein, we present an unprecedented experimental demonstration and structure-property relationship on coherent exciton dynamics and its related vibrational signatures of columnar dye stacks with their H-type exciton coupling. Supramolecular dye assemblies have received attention as a medium for the efficient transport of excitons and charge carriers for widespread applications in artificial light-harvesting systems, organic photovoltaics, and organic solar cell. In this context, supramolecular model systems facilitate unveiling appearing functionalities not seen in its constituent molecules. In sharp contrast with stacks with J-type exciton coupling, however, the detailed observation of exciton dynamics in H-type aggregates has remained challenging because of the small oscillator strength of the Frenkel state and the weak fluorescing nature of the energetically lower-lying state. Using femtosecond transient absorption and time-resolved impulsive stimulated Raman scattering measurements, we succeed in observing the excited state dynamics of self-assembled perylene bisimide (PBI) H-aggregates in two points of view: a) the intermolecular interactions between PBI units in H-aggregates induce the formation of new excited-states, excimer and delocalized radical anion states, and b) the intermolecular out-of-plane along the stacking axis and the PBI core C=C stretch Raman modes can be vital evidence to grasp the coherent exciton dynamics in H-aggregates.

Poster Presentation : **PHYS.P-68**
Physical Chemistry
Event Hall THU 11:00~13:00

Mitochondrion-Targeting PEGylated BODIPY Dyes for Near-Infrared Cell Imaging and Photodynamic Therapy

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Photodynamic therapy (PDT) is a promising cancer treatment for its variety advantages such as non-invasive and controllable characteristics. A 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY) has been extensively studied as a potential PDT agent due to its excellent advantages such as high extinction coefficients and good photostability. Herein, we synthesized a series of BODIPY-based photosensitizers (PSs) (AmB*X*I, *X* = H, M, Br) featuring a cationic mitochondrion-targeting group and near-infrared (NIR) absorption. The absorption wavelength shifted to the phototherapeutic wavelength range (650–900 nm) through the extending the PS's π–π conjugation via Knoevenagel reaction. Theoretical data demonstrate that the introduction of bromine atoms facilitates the intersystem crossing (ISC) via heavy atom effect, so that for each additional bromine atom in AmB*X*I an increase in singlet oxygen quantum yield would be expected (0.3%, 2.2%, and 4.1%, for AmBHI, AmBMI, and AmBBrI, respectively). Moreover, AmB*X*I PSs exhibited low cytotoxicity in the dark and high phototoxicity, with the half maximal inhibitory concentrations of AmBBrI found to be 46.93 nM and 22.84 nM, while those of AmBMI were 129.7 nM and 58.34 nM in HeLa and MCF-7 cancer cells, respectively. Notably, introduction of a single bromine atom was enough to produce a cytotoxic effect. Furthermore, the presence of a quaternary ammonium group in AmB*X*I enabled the dyes to localize and stain the negatively charged mitochondria. Overall, we were successfully synthesis of NIR-absorption mitochondrion-targeting BODIPY-based PSs. All the results herein will great contribution to development of strategy for designing novel PSs applicable for practical cancer therapy.

Poster Presentation : **PHYS.P-69**

Physical Chemistry

Event Hall THU 11:00~13:00

Anisotropic circular dichroism spectroscopy of jet-cooled chiral molecules

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Circular dichroism (CD) spectroscopy is one of the most powerful methods to investigate the structures and reactions of chiral molecules. The CD of molecules with fixed spatial distribution is called anisotropic CD (ACD). ACD spectroscopy has been extensively used to probe the orientation of macromolecules in anisotropic medium. Here, we have obtained the resonant two photon ionization CD (R2PI-CD) spectra of rotational P-, Q-, and R-branch transitions for the origin bands of conformers A, B, and C of (−)PED using a dual laser beam method. It is found that the CD values of the P-, Q-, and R-branch transitions of the origin bands are different from each other. Furthermore, the CD values of the rotational transitions of conformers A and C do not exhibit mirror images between (+) and (−)PED. These results are explained by ACD phenomena of jet-cooled molecules undergoing the P-, Q-, and R-branch transitions.

Poster Presentation : **PHYS.P-70**

Physical Chemistry

Event Hall THU 11:00~13:00

Study on the binding affinity of Leucosporidium-derived ice-binding protein (LeIBP) using steered MD simulation

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Ice-etching experiment and molecular docking demonstrated that Leucosporidium-derived ice-binding protein (LeIBP) from artic yeast, shows suppression of the growth and re-crystallization of ice, leading to a thermal hysteresis (TH). In this study, we investigated the ice-binding pattern of the LeIBP to ice plane using steered molecular dynamics simulation.

Poster Presentation : **PHYS.P-71**
Physical Chemistry
Event Hall THU 11:00~13:00

Trapping Alkali Halide Cluster Ions in the Cucurbit[n]uril During the Solvent Evaporation

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Trapping molecules inside the tiny nano-sized molecular cavity have received significant attention both experimentally and theoretically. Especially, cucurbit[*n*]uril is one of the extremely efficient molecules to exhibit host-guest chemistry with metals, organic and biomolecules. Its extensive host properties have been applied to various industries by capturing targeted molecule. Therefore, understanding pathway of confining the molecules inside the cavity is the fundamental question to be solved for further application. In the present work, CB[7]-alkali chloride cluster cations and anions generated via rapid solvent evaporation during the electrospray ionization were investigated by ion mobility spectrometry-mass spectrometry (IMS-MS) which enables us to determine whether the complex cluster ions form inclusion complexes. Based on the collision cross section (CCS) values of CB[7]-alkali halide cluster ions obtained by IMS-MS, cluster ions up to certain critical cluster size (m) were revealed to be trapped in the CB cavity, even though it is thermodynamically unfavorable for salt clusters to penetrate into the cavity. Furthermore, the maximum cluster size trapped inside the cavity shows the strong dependence on the ionic diameter of alkali metal species. Theoretically, the structures of several stable inclusion complexes were predicted by density functional theory (DFT) calculations. The possible driving force for the cluster trapping were theoretically investigated by molecular dynamics (MD) simulations as well. We expect the present results may further provide a new way to investigate the encapsulation of various atomic clusters in the diverse host molecules with cavity.

Poster Presentation : **PHYS.P-72**

Physical Chemistry

Event Hall THU 11:00~13:00

$\mathrm{Li^+}$ and $\mathrm{Li^+I^-Li^+}$ Ions Solvated by 1,4-dioxane: An Ion Mobility Spectrometry-Mass Spectrometry Study

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Electrolyte solution contains the number of ionic and neutral species, and the species form contact ion pairs under the high concentration. These ions and ion pairs can be solvated by neutral solvent molecules, and investigating these complexes is important because they have a great influence on ion transport properties. In the present work, we investigated $\mathrm{Li^+}$ and $\mathrm{Li^+I^-Li^+}$ ions solvated by 1,4-dioxane using ion mobility spectrometry-mass spectrometry (IMS-MS). LiI solution was electrosprayed under the presence of the 1,4-dioxane vapor, which enabled $\mathrm{Li^+}$ and $\mathrm{Li^+I^-Li^+}$ to form solvated complex ions with 1,4-dioxane molecules in the gas phase. Several $(\text{1,4-dioxane})_m\cdot\mathrm{Li^+}$ complex ions (m = 1, 2, and 3) and a $(\text{1,4-dioxane})\cdot\mathrm{Li^+I^-Li^+}$ complex ion were observed by MS, and furthermore the presence of their structural isomers was confirmed by IMS. The collision cross section (CCS) values obtained from IMS were used to predict the structures of the observed isomers with help of the density functional theory (DFT) calculations. The thermodynamic stabilities of the predicted isomers were compared as well. Our results suggested that the conformation and the denticity of 1,4-dioxane are major factors governing the stability of the $\mathrm{Li^+}$ and $\mathrm{Li^+I^-Li^+}$ solvated by 1,4-dioxanes. This research clearly demonstrates that the isomer-specific approach is mandatory for investigating the solvated ions and electrolytes.

Poster Presentation : **PHYS.P-73**
Physical Chemistry
Event Hall THU 11:00~13:00

Nonadiabatic Molecular Dynamics Study on the Ultrafast Photoisomerization of 1,2-Dihydro-1,2-azaborine

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Ultrafast dynamics of the organic molecules is getting popular among chemists, due to its novelty and wide applicability in the frontier of the chemistry research field. However, simulation of the photoexcited organic molecule has some obstacles, the complexity of the dynamics itself and the cost of the computations containing many near-degenerate excited states. Therefore, investigating the excited state behavior of the small organic molecules are important as the analogous manner of the large and complex systems. One example of the small but important molecules in terms of the excited states dynamics is the 1,2-dihydro-1,2-azaborine (hereinafter referred to as azaborine), which is the isoelectronic to benzene, replacing one of the C-C bonds to the B-N bond. Previous research reported that UV irradiation of 253.7 nm wavelength converted azaborine into Dewar form (2-aza-3-borabicyclo[2.2.0]hex-5-ene) [1], and the photoexcited isomerization pathway was investigated theoretically [2]. However, total conversion of the azaborine was not explained well due to the lack of the excited states dynamics result. In this research, nonadiabatic molecular dynamics on the azaborine system was conducted using the surface hopping algorithm. Among the 80 trajectories propagated in 500 fs, 2 trajectories show the conversion to the Dewar form, while the 69 trajectories choose to fall back to its original form. From the result, we can confirm the expectation from the previous PES investigation, that only the small portion of the excited population reaches the Dewar form due to the slope of the branching space near conical intersection structure.Reference[1] Brough, S. A. et al., Angew. Chem. Int. Ed., 51, 10880–10883 (2012).[2] Kim, J. et al., ChemPhysChem, 16, 1670-1675 (2015).

Poster Presentation : **PHYS.P-74**

Physical Chemistry

Event Hall THU 11:00~13:00

High-resolution vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of 3-fluoropyridine

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We measured the cationic vibrational spectrum of 3-fluoropyridine (3-FP) using high-resolution one-photon vacuum ultraviolet mass-analyzed threshold ionization (HR VUV-MATI) spectroscopy adopting the intense VUV laser pulse generated by four-wave difference frequency mixing in the Kr gas. The HR vibrational spectrum, which is obtained from the zero-point energy level of the 3-FP cation via a direct adiabatic ionization transition from the vibrational ground state of the neutral molecule, is comprehensive of the adiabatic ionization energy of the neutral molecule. Based on the 0-0 band in the HR VUV-MATI spectrum, the adiabatic ionization energy of 3-FP was determined to be 9.5335 ± 0.0004 eV (76593 ± 3 cm^{-1}), which is much higher but more accurate than the previous value of 9.49 eV by the tho-photon MATI spectroscopy. Notably, many vibrational peaks with higher intensities than that of the 0-0 band were observed in the spectrum, implying that the cationic geometry was largely changed upon ionization with respect to the neutral geometry. The quantum chemical calculations show that the cationic geometry has a C$_1$ symmetry rather than C$_S$ symmetry for the neutral geometry.

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Poster Presentation : **PHYS.P-75**

Physical Chemistry

Event Hall THU 11:00~13:00

Searching for the Liquid-Liquid Critical Point in supercooled water with the two-laser heating of amorphous ice

Seonju You, Kyung Hwan Kim*

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Water is the most important liquid for our existence and it has unique anomalous behavior of many of its macroscopic properties. One of the most important topics in physics and chemistry is what causes this anomalous behavior. One major hypothesis is that there could exist two separate macroscopic liquid water phases, high-density liquid (HDL) and low-density liquid (LDL), with a coexistence line in the P-T diagram deep in the supercooled regime at elevated pressure. This liquid-liquid transition (LLT) line is proposed to end in a liquid-liquid critical point (LLCP) and its extension into the one-phase region corresponds to the Widom line. If the LLCP exists in “no-man’s land”, the discontinuity due to the LLT would disappear at high enough temperatures and only a continuous transition would be observed with a maximum at the Widom line. To investigate supercooled water in the “no-man’s land”, we measured ultrafast heating from glassy high-density amorphous ice (HDA) state into the HDL and then follow how it transforms to the LDL state (HDA→HDL→LDL). We got direct evidence of LLT from a previous PAL-XFEL beamtime experiment. However, we were not able to obtain high enough temperature jump (T-jump) to reach up to the potential LLCP and Widom line even at the highest base temperature, 115 K. So, the measurements with higher T-jump are desired to observe LLCP experimentally. In this experiment done in PAL-XFEL, we use two lasers to achieve high enough T-jump. A nanosecond laser system (up to ~2 mJ at 2 μm) is used as a pre-heating source and a femtosecond laser system (up to 90 mJ/mm^2 at 2 μm) is used as a pump for ultrafast T-jump.

Poster Presentation : **PHYS.P-76**
Physical Chemistry
Event Hall THU 11:00~13:00

Determination of the highest occupied molecular orbital and the cationic structure of 3-chloropyridine using high-resolution VUV-MATI mass spectroscopy

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Pyridine, which is a basic nitrogen-containing heterocycle found in various natural products, has stimulated interest in many physical chemists because of alteration in the highest occupied molecular orbital (HOMO) of the aromatic molecule. Various experimental and theoretical studies regarding the photophysical and photochemical properties of pyridine are now convinced that two outermost orbitals, a nonbonding orbital of lone-pair electron on nitrogen atom and a π orbital of aromatic ring are closely lying. Recently, we are interested that the substitution of the halogen atom with the H in pyridine alters the HOMO of the molecule but the HOMO of halopyridine except for 2-chloropyridine was rarely studied. Therefore, we measured the cationic vibrational spectra of 3-chloropyridine (3-CP) having ^{35}Cl and ^{37}Cl using the high-resolution vacuum ultraviolet mass-analyzed threshold ionization (HR VUV-MATI) mass spectroscopy. Based on the origin band in the VUV-MATI spectrum of 3-CP with ^{35}Cl, the adiabatic ionization energy of 3-CP was determined to be 9.4058 ± 0.0004 eV with a similar value for ^{37}Cl, which is similar but more accurate than the previous value of 9.40 eV by the two-photon MATI spectroscopy. Then, we found that the spectral feature for 3-CP is similar to that of 2-CP, unlike pyridine, implying that the HOMO of 3-CP probably consists of the π orbital in the pyridine ring, like 2-CP. We are performing the quantum chemical calculations to analyze the measured VUV-MATI spectra of 3-CP, which will draw a conclusion regarding the HOMO and the cationic structure of 3-CP.

Poster Presentation : **PHYS.P-77**

Physical Chemistry

Event Hall THU 11:00~13:00

Determination of the molecular orientation during the wavepacket motion using anisotropic time-resolved x-ray Liquidography

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Photoselective alignment of molecule produced by linearly polarized laser pulse creates an anisotropic x-ray scattering signal. Since laser pulse preferentially excites the molecules with the transition dipole moments parallel to the laser polarization axis, this anisotropy contains information on molecular orientation with respect to the transition dipole moment of the molecule. In this study, we present a quantitative analysis of the anisotropic part of the time-resolved x-ray liquidography (TRXL) signal, based on the structural dynamics obtained by azimuthal integration of the scattering signal. We analyzed anisotropic part of the TRXL signal arise from the wavepacket motion of the gold trimer complex, $[Au(CN)_2^-]_3$. Molecular orientation of the gold trimer complex during the wavepacket motion was tracked and showed that anisotropic scattering signal can add structural sensitivity compared with isotropic scattering signal.

Poster Presentation : **PHYS.P-78**

Physical Chemistry

Event Hall THU 11:00~13:00

Revealing a hypothetical fragile to strong transition in deeply supercooled water using anisotropic X-ray scattering under Optical Kerr Effect condition

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Most liquids can be classified into two categories, fragile and strong ones, depending on their temperature dependence of the dynamics. Water at ambient temperature and modest supercooled conditions is considered to be a fragile liquid whereas it is proposed to be a strong liquid at temperatures close to the glass transition, which is 135 K. Thus, it is postulated that there exists a fragile to strong transition somewhere in the deeply supercooled regime. By time-resolved X-ray scattering under Optical Kerr Effect (OKE) condition and evaporative cooling in a vacuum can give a chance to find those properties. For the OKE scattering measurement on supercooled water at PAL-XFEL, we have built the equipment that can generate deeply supercooled water droplets and have successfully tested it down to ~227 K. From the recent experiment at PAL-XFEL, we have measured time-dependent anisotropy signal of liquid water induced by strong electric field down to ~235 K.References1) C.A. Angell, Science 319, 582-587 (2008). 2) J. A. Sellberg et al., Nature 510, 381-384 (2014)3) K. H. Kim et al., Phys. Rev. Lett. 125, 076002 (2020)

Poster Presentation : **PHYS.P-79**
Physical Chemistry
Event Hall THU 11:00~13:00

Time-resolved photoelectron experiment of cryogenic nitromethane anion photodetachment dynamics

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The anion photodetachment dynamics has been explored with a pump-probe experimental technique. Especially, a pump-probe experiment with the picosecond laser has the advantage of revealing the state-resolved and time-resolved anion dynamics. Vibrational excitation by pump pulse initiates the reaction and several picoseconds after the pump enters, probe pulse can detach the electron from the intermediate anion of the reaction. As the ps time delay between the pump and probe pulse varies, the information of detached photoelectron changes.Normally. anion source, mass selection system, VMI photoelectron spectrometer, and picosecond laser system should be prepared for this pump-probe experiment. For cryogenic anion photoelectron spectroscopy, the new design of the spectroscopy apparatus is needed. In our apparatus, a closed-cycle cryostat is mounted on a copper quadrupole ion trap (QIT). The anions are guided into the QIT through the einzel lens and trapped inside the trap for tens of ms. While the anion is trapped, the temperature of the anion becomes cryogenic by collisional cooling with Helium buffer gas. The cryogenic anion enables us to observe vibration-controlled reaction dynamics.The first target system is the nitromethane anion photodetachment dynamics. The time-resolved photoelectron experiment for the nitromethane anion has not been researched by using the picosecond laser pulse. We expect that the autodetached rate from the nitromethane anion can be measured. By comparing the autodetachment rate for the specific vibrational mode, we will be able to reveal the vibration mediated autodetachment dynamics of ground state nitromethane anion.

Poster Presentation : **PHYS.P-80**

Physical Chemistry

Event Hall THU 11:00~13:00

A Molecular Dynamics Simulation Study for Polarization effects on Organic Ionic Plastic Crystals

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The organic ionic plastic crystals (OIPCs) have been considered as a strong candidate for the solid electrolytes of all solid-state batteries. Ordinary solid electrolytes exhibit low ionic conductivity due to restricted molecular motions. However, ions in OIPCs may rotate while they maintain a long-range ordered crystalline lattice structure. Such rotational motions facilitate the diffusion of dopant ions, which enhances the conductivity. Some rotational motions of ions in OIPCs are activated at a certain temperature range and result in multiple solid rotator phases. Activated molecular rotational motions enhance conductivity. Therefore, investigating the rotational motions of ions in OIPCs at a molecular level is important. Molecular simulations are successful approaches, but polarization effects were often ignored in the previous studies because of high computational costs. In this work, we investigate how the polarization effects affect the rotational diffusion of ions in OIPCs. We perform atomistic molecular dynamics simulations of 1-methyl-3-methylimidazolium hexafluorophosphate ([MMIM][PF_6]) at temperatures from 75 to 500K under NPT conditions with and without electronic polarization. Polarization has little impact on density and structure of [MMIM][PF_6] crystals. However, polarization induces a faster rotational relaxation. PF_6^- ions undergo up to four times faster rotation with polarization considered. This suggests that polarization affects the rotational dynamics of ions in OIPCs significantly, which may enhance the diffusion and the conductivity of dopants in OIPCs.

Poster Presentation : **PHYS.P-81**

Physical Chemistry

Event Hall THU 11:00~13:00

Role of Vacancies in Phase Change Materials

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Phase change materials are widely used as memory devices, but the mechanism is still unclear. The vacancy in the van der Waals layer is experimentally known to play an important role in the function of the phase change materials. Analyzing the dynamics of vacancies is a difficult task in experiments, but it can be easily solved by calculating electronic structures using density functional theory. This work shows that the mechanism in Sb_2Te_3 can be explained through the concept of "positively charged vacancies". In particular, the dynamics of the vacancies in $GeTe_2/Sb_2Te_3$ cause a decisive change in the chemical state of Ge and consequently significant changes in the electrical resistance.

Poster Presentation : **PHYS.P-82**

Physical Chemistry

Event Hall THU 11:00~13:00

The Molecular Dynamics Simulation Study of the Difference in Membrane according to CSLs' Concentration

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Chlorosulfolipids (CSLs) are lipids of flagellar membranes in sea algae. They are toxic and are known to be related to Diarrhetic shellfish poisoning. CSLs have various structural isomers, with a charged sulfate group in the middle of the hydrophobic chain. In this study, we used Danicalipin A as a CSL and dipalmitoyl-glyceryl-trimethylhomoserine (DPTS) as a glycerolipid and performed coarse-grained (CG) simulation and atomicstic molecular dynamics (MD) simulation to gain difference in mixed system with membrane, which is a rare class of glycerolipid that is found in Ochromonas Danica. We observed that CSL molecule's position and shape are same as Frank's model(2020)[1] of the CG simulation. Based on these CG MD results, we additionally performed MD simulation of the corresponding atomistic model.

Poster Presentation : **PHYS.P-83**

Physical Chemistry

Event Hall THU 11:00~13:00

Structural Stability of Mutated Lignin Peroxidase: Molecular Dynamics Simulation Studies

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Lignin is an abundant aromatic biopolymer found in the lignocellulos component of the plant cell wall. The lignin peroxidase isozyme H8 from white-rot fungus *Phanerochaete chrysosporium* (PcLiP01) is one of the most widely studied isozymes which can degrade lignin via oxidative mechanisms. Denaturation caused by heat and pH is still a great issue in enzyme studies. Recently, it was observed that the melting temperatures rose in several single mutants of PcLiP01, especially in the V181A mutant model. A triple mutant (E40S/G86I/V181A) showed significant improvement of Tm in pH 3.0. It was conjectured that this effect would be attributed to the newly formed interactions between the heme and the mutated residues. In this study, we performed Molecular Dynamics (MD) simulations with both wild type (WT) and triple mutant (MT) PcLiP01. The stabilities of secondary structures which are related to the mutated residues were investigated during the simulation. Interactions around residue 181 indicated notable differences between WT and MT, which is consistent with experimental observation. These results demonstrate that the structural stability of lignin peroxidase is affected by the mutation of residues in secondary structures.

Poster Presentation : **PHYS.P-84**

Physical Chemistry

Event Hall THU 11:00~13:00

Machine-Learning XC Functional improved by targeting decomposed error

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In modern computational chemistry, Kohn-Sham density functional theory (KS-DFT) is the standard method for theoretical studies of the properties of the molecules. However, since the exchange-correlation (XC) functionals from the practical KS-DFT are approximated, the error called total error occurs which is the energy difference from the exact KS-DFT. The total error can be decomposed into two components: density-driven error and functional error. These two types of error, the XC functionals constructed with the total error as a target have difficulties in describing the physical properties. These XC functionals are suffered from the blended effect between density-driven error and functional error which can be seen as a collapse for the response function of the energy. In this presentation, the machine learning technique is used to create an XC functional that targets decomposed errors for the flexibility of the functionals.

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Poster Presentation : **PHYS.P-85**

Physical Chemistry

Event Hall THU 11:00~13:00

Binding Interaction between JMJD2A(KDM4A) and Its Substrates: Molecular Dynamics Simulation Studies

Jiyeon Hyun, Rakwoo Chang*

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JMJD2A (jumonji domain containing 2A) is a JmjC histone demethylase that catalyzes the demethylation of di- and tri-methylated Lys9 and Lys36 in histone H3 (H3K9me3/me2 and H3K36me3/me2). The catalytic domain of human JMJD2A bound to Fe (II) and 2-oxoglutarate (2OG) has been resolved by crystallographic analysis. Recently, the structural similarity of the JmjC domain between FIH-1 containing histone lysine dimethylases (JmjC-KDMs) and histone Jumonji C domain was studied in anticipation that Clioquinol (CQ) could inhibit the catalytic activity of JmjC-KDMs. In this study, we have performed molecular dynamics simulations of JMJD2A with several substrates including 2OG, CQ and pyridine-2,4-dicarboxylic acid (PDCA) with known crystal structure expected to have an active site at a position similar to CQ. The structural and dynamic stability of each substrate at the active site were examined. The results showed that 2OG, CQ, and PDCA were competitive, which supports the notion that CQ can inhibit the catalytic activity of JmjC-KDMs.

Poster Presentation : **PHYS.P-86**

Physical Chemistry

Event Hall THU 11:00~13:00

Field-induced Radial Junction for Dopant-free Crystalline Silicon Microwire Solar Cells with an Efficiency of Over 20%

Deokjae Choi, Kwanyong Seo*

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Radial junctions on crystalline silicon (c-Si) microwire structures considerably reduce the diffusion length of photo-induced minority carriers required for energy generation by decoupling light absorption and carrier separation in orthogonal spatial direction. Hence, radial junctions mitigate the need for high-purity materials, and thus reduce the fabrication cost of c-Si solar cells. In this study, the formation of dopant-free radial junctions from atomic layer deposition (ALD) of Al2O3 on an n-c-Si microwire surface is reported. ALD-Al2O3 generates a p+ inversion layer, which eventually forms the radial junction on the n-c-Si surface. The width of depletion region induced by the p+ inversion layer is calculated from PC1D simulation as 900 nm. The fabricated dopant-free radial junction c-Si solar cells exhibits a power conversion efficiency of 20.1%, which is higher than those of previously reported microwire-based radial junction solar cells. Notably, internal quantum efficiencies of over 90% were obtained in the 300–980 nm wavelength region, thereby verifying the successful formation of radial junctions.

Poster Presentation : **PHYS.P-87**

Physical Chemistry

Event Hall THU 11:00~13:00

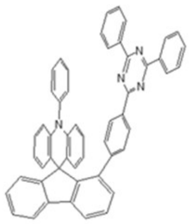
A theoretical study of Donor-Bridge-Acceptor type thermally activated delayed fluorescence (TADF) molecules

Kanghyeon You, Dongwook Kim[1,*]

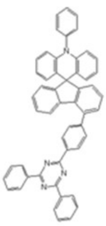
Kyonggi University, Korea

[1]*Department of Chemistry, Kyonggi University, Korea*

A theoretical study of Donor- Bridge-Acceptor type thermally activated delayed fluorescence (TADF) moleculesIn organic light emitting diodes (OLEDs), singlet and triplet excitons are generated at 1:3 ratio via the charge recombination.[1]Therefore, to make OLEDs efficient, triplet excitons should be harnessed in light emission. Highly efficient devices can be manufactured based on thermally activated delayed fluorescence (TADF) emitters. These emitters can be purely organic and fully exploit triplet excitons by converting them to singlet ones.[2] In this regard, TADF OLEDs have attracted a great deal of attention. Recently, interest in exciplex-type TADF molecules is rapidly growing.[3],[4] In this sense, we studied the Donor-Bridge-Acceptor Type of TADF molecules, where donor and acceptor units are either in exciplex-like face-to-face conformation or conventional head-to-tail conformation. We took 10-phenyl-9,10-dihydroacridine, 2,4,6-triphenyl-1,3,5-triazine, and fluorene as donor, acceptor, and bridge units, respectively.[4] Due to the electron correlation, we employed Algebraic Diagrammatic Construction (2) [ADC(2)] methodology in geometry optimization and gap-tuned range-separation density functional theory (DFT) functional in electronic structure calculation. By conducting various theoretical analyses, we compare exciplex-like and conventional D-A type TADF molecules. References[1] S. S. Kothavale et al. Adv. *Opt. Mater*. 18, 2000922 (**2020**)[2] Yang, Z. Y. et al. *Chem. Soc. Rev*. 46, 915 (**2017**)[3] Sheng-Yi Yang, et al. *J. Am. Chem. Soc*. 142, 17756 (**2020**)[4] Tang, et al. *Nat. Mater*. 19, 1332 (**2020**)



1'-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-10-phenyl-10H-spiro[acridine-9,9'-fluorene]



4'-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-10-phenyl-10H-spiro[acridine-9,9'-fluorene]

Poster Presentation : **PHYS.P-88**

Physical Chemistry

Event Hall THU 11:00~13:00

Quantitative evaluation of fluorescent nanoparticle brightness using DNA origami standards

Sihwa Joo, Tae geol Lee[1], Mina Lee[1,*]

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[1]*Safety Measurement Institute, Korea Research Institute of Standards and Science, Korea*

Fluorescent nanoparticles (FNP) have been widely used in bio-sensing and bio-imaging since particles with a wide range of sizes are available, and various types of ligand can be introduced. Target binding of the FNP is monitored by the fluorescence brightness. Unfortunately, the brightness of FND is considerably different depending on the size and synthesis method. There is a large particle-by-particle variance in brightness among the same FNP. However, techniques, which can quantitatively evaluate the brightness of FNP, are still lacking. Here, we present a method to assess the brightness of FNP using DNA origami standards, a series of DNA nanostructures labeled with the defined number of dyes. When the origami standards were imaged with a total internal reflection microscope, their brightness was linearly proportional to the number of labeled dyes. By comparing the brightness of FNP with those of origami standards, we determined the average brightness of FNP and particle-by-particle variation. We applied this method to two commercial FNP and found that their brightness corresponded to that of 10 - 15 dye molecules and intensity distribution was much broader than the origami standards.

Poster Presentation : **PHYS.P-89**

Physical Chemistry

Event Hall THU 11:00~13:00

Methods to Determine Layer Numbers and Measure Properties of MoS_2

Jehyun Oh, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

MoS_2 is one of the two-dimensional semiconducting transition-metal dichalcogenides. MoS_2 has different band gap determined by the number of layers of MoS_2 and grain shape depending on the concentration of the precursor. Therefore, it is important to know which methods to analyze MoS_2 and to know the number of layers accurately also.In this poster, methods for determining the number of layers will be compared and various methods for analyzing MoS_2 will be described. Methods for determining the number of layers include thickness measurement using atomic force microscopy (AFM), a method of looking at the peak difference between A_{1g} and E^1_{2g} of Raman spectra, a method of comparing the intensity of photoluminescence spectra of MoS_2, and contrast method using specific wavelength light source with a 285 nm thickness of SiO_2 substrate. Contrast measurement is the easiest method to measure without affected by the roughness and strain of the substrate.The method of analyzing MoS_2 can be divided into analysis methods according to the sources to be entered. There are a scanning electron microscope and a transmission electron microscope that can analyze the surface using electrons. Using back scattered electron, selected area electron diffraction and electron backscatter diffraction methods can determine the crystal structure. Analysis using X-rays includes X-ray diffraction and X-ray photoelectron spectroscopy. As for the tip scanning method, there are AFM and conductive AFM that can know electric properties, electrostatic force microscopy that can know piezoelectric properties, and scanning tunneling microscopy with atomic resolution using tunneling current.

Poster Presentation : **PHYS.P-90**

Physical Chemistry

Event Hall THU 11:00~13:00

Direct observation of distinct amyloid aggregation dynamics: Use of 2D-IR spectroscopy and IR microspectroscopy

So Yeon Chun, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

Amyloid proteins that undergo self-assemblies to form insoluble fibrillar aggregates have attracted much attention due to their role in biological and pathological significance in amyloidosis. Various spectroscopic techniques, including infrared (IR) spectroscopy, have made efforts to trace the appropriate structural dynamics indicative of the complex mechanisms of the aggregation process. However, IR studies are limited in water (H_2O) by the signal overlap of H-O-H bending mode of H_2O and amide I band and are done in heavy water (D_2O), which raises fundamental questions regarding the isotopic effect of D_2O on protein dynamics. In a previous study, we have tracked the different amyloid aggregation dynamics of insulin (INS) in H_2O and D_2O using two-dimensional IR spectroscopy (2D-IR) and various biophysical tools. Utilizing the advantages of 2D-IR, we could directly monitor the structural changes during INS fibrillation and reveal that the unique quaternary structure of INS causes distinct fibrillation pathways in two water solvents. In subsequent studies, we use IR microspectroscopy to aim to better understand the pathogenic factors for liquid-liquid separation (LLPS)-mediated fibrillation processes at the molecular level beyond the effects of solvents. Studies on LLPS-mediated fibrillation has recently received attention because of its role in inducing aggregation. In addition, it is known that LLPS is formed in the nucleation process, which is an initial stage of fibrillation, and toxic oligomers are generated at this time. We confirmed the possibility of tracking the LLPS-mediated fibrillation using IR microspectroscopy.

Poster Presentation : **PHYS.P-91**

Physical Chemistry

Event Hall THU 11:00~13:00

Synthesis and Phase Evolution in tin-based Halide Perovskite Quantum Dots using Temperature-controlled Ultra-Low Frequency Raman Spectroscopy.

Jiwon Choi, Myeongkee Park*, Nurwarrohman Andre Sasongko, Jaeseong Heo, Donggyu Kim

Department of Chemistry, Pukyong National University, Korea

Formamidinium tin iodide (FASnI3, FA+: CH[NH2]2+) is a promising candidate for long-term solar energy harvesting and other optoelectronic applications. Compared to lead-based bulk and quantum dot (QD) perovskites, lead-free FASnI3 quantum dots can be used for environmentally favored solar cell applications. FASnI3 quantum dots can be easily synthesized by using the hot injection method, but easily degradable. Thus, in order to increase the low stability of FASnI3 QDs in the ambient condition, it requires more studies of structure, temperature-dependent phase transition, and degradation pathways, which are not clearly determined yet. In this work, we will present the first Raman study of FASnI3 QDs using ultra-low Frequency Raman microscopy (

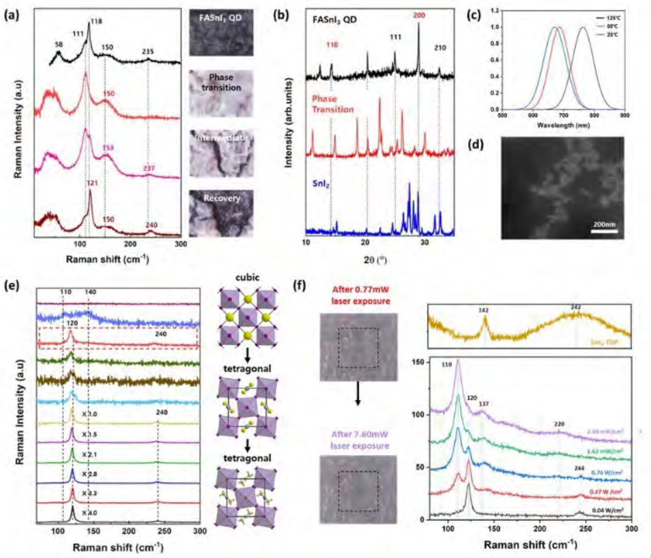


Figure 1. **(a)** Schematic of FASnI$_3$ phase transition driven by humidity, and the raman spectrum of each phases, FASnI$_3$ nanocrystals (black), transition phases (red), intermediate phases (pink), recovered phases (brown), **(b)** XRD patterns for the FASnI3 nanocrystals (black), transition phases (red) and SnI$_2$ phases (blue), **(c)** Steady-state photoluminescence measurements of FASnI$_3$ nanocrystals with different growth temperature, **(d)** A TEM image of the crystal structure of the cubic phase FASnI$_3$ (scale bar, 200 nm), **(e)** Schematic of FASnI$_3$ phase transition from tetragonal phases (P4/mbm) to the cubic (Pm3m) phases in the temperature range of 300 to 85 K, **(f)** Schematic of photo -induced phase transition of FASnI$_3$.

Poster Presentation : **PHYS.P-92**
Physical Chemistry
Event Hall THU 11:00~13:00

The theoretical study of bond dissociation energies (BDEs) and rates

Hyeong seon Park, Dongwook Kim*

Department of Chemistry, Kyonggi University, Korea

Organic light emitting diodes (OLEDs) are widely used for TV, monitor, and large area solid-state displays. Recently, thermally activated delayed fluorescence (TADF) OLED devices have been studied; they can reach the internal quantum efficiency (IQE) of nearly 100% by upconverting triplet excitons to emissive singlet excitons,[1] while they can be fabricated at much lower cost compared to phosphorescence OLED (PhOLED).[2]Although highly efficient TADF OLEDs continue to be reported, issues regarding the device lifetime still needs to be solved. Such device lifetime is known to be closely related to the chemical stability of organic semiconducting molecules. In particular, the degradation of an emitter molecule is largely responsible for the impediment of operation OLED devices, because its excitation energy can promote the dissociation of relatively weak bonds,[3] and due to their higher energy, blue emitters are more vulnerable to such bond dissociation than red or green emitters.[4] Over the past few years, a few studies have been carried out regarding such bond dissociations of organic semiconducting materials. However, studies as to how effectively and efficiently such bonds dissociate have rarely been reported. As for representative organic semiconducting materials for OLEDs applications, we investigated the bonds that are possibly broken during the device operation at density functional theory (DFT) level. Then, we calculated the dissociation energies and rates[5] of such bonds. We believe this study will allow us to provide a fundamental insight into the relationship between molecular structure and the chemical stability of organic semiconducting materials.[1] Huifang Li, Minki Hong et al. Chem. Mater. 2019, 31, 5, 1507–1519[2] Man-chung Tang, Mei-Yee Chan et al. Chem. Rev. 2021, 121, 7249−7279[3] Minki Hong, Mahesh Kumar Ravva et al. Chem. Mater. 2016, 28, 5791−5798[4] Chao Deng, Siyu Zheng et al. J. Phys. Chem. C 2019, 123, 29875−29883[5] J. Zheng, J. L. Bao D. G. Truhlar et al. Gaussrate 17, University of Minnesota, Minneapolis, MN, 2017.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-93**

Physical Chemistry

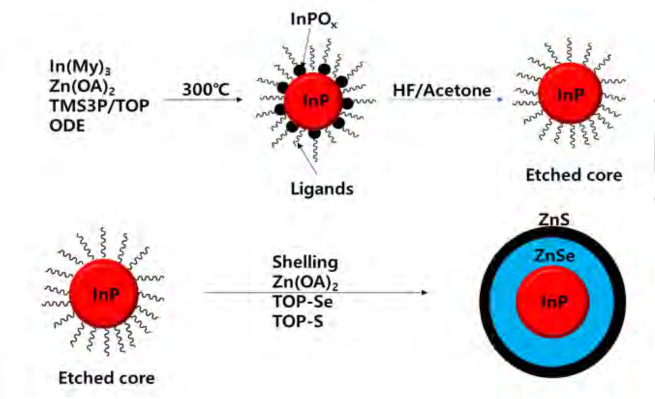
Event Hall THU 11:00~13:00

Development of environmentally benign red, and green InP/ZnSe/ZnS quantum dot (QD).

Younghee Park[*], Suntae Hwang, Bongmin Choi

Semiconductor Division, ODTECH, Korea

The ecofriendly InP-based QDs become alternative to Cd-based QDs and replacing its applications as well. The QDs can be tuned with various emission wavelength by changing the size of the QDs. In addition, the QDs possesses outstanding color purity, narrow band width, photostability, and high quantum yield making them as a new exploring material for display and other applications. The decade of research, the synthetic methods and the properties of InP QDs have been developed and improved performance of the InP-based QLEDs. The proper passivation of InP improve its stability and other properties. The InP QD with higher PLQY of 90% and lower FWHM is the basic requirement for industrial applications.



Poster Presentation : **PHYS.P-94**

Physical Chemistry

Event Hall THU 11:00~13:00

The effect of chain flexibility and the fraction on the spatial distribution and diffusion of the thin film of blends of ring and linear polymers

Jong Ho Choi, Bong June Sung*

Department of Chemistry, Sogang University, Korea

When mixing two polymers, the interaction energy between them and their fraction determine the miscibility of the blends. However, at the surface of films, entropy difference originated from flexibility or topology of chains can also drive non-homogeneous distribution. In this work, we find the effect of flexibility of polymer chains on the spatial distribution of films of polymer blends with the same interaction energy but different topology (ring and linear polymers) by performing molecular dynamics simulations. To examine whether the effect depends on the fraction of the blends, we mixed ring and linear polymers of different flexibility in various fraction. We find the relative flexibility differences between the ring and linear chains determines where each chain prefers to be located that for all the fractions of blends we have observed. The more flexible (stiffer) chains prefer to be at the surface (center) of the film. However, how strong the surface preference of the chains depends on the fraction of blends. While a relatively flexible ring polymer chain of the lowest fraction ($\phi_{ring} \cong 0.008$) is five times more likely to be at the surface than at the center, the same flexible ring of ϕ_{ring} =0.5 is only 1.5 times more likely to be at the surface. The fraction of rings also affects the number of threading of linear chains through the ring chains significantly. The number of threading linear chains decreases with increasing ring fraction, so the ring chains of higher fraction diffuse faster than the rings of lower fraction.

Poster Presentation : **PHYS.P-95**

Physical Chemistry

Event Hall THU 11:00~13:00

Computational studies on ion conduction mechanisms in 1,3-dimethylimidazolium hexafluorophosphate

Hyungshick Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystals (OIPCs) are molecular crystals which consist of bulk cations and anions. These OIPCs show not only plastic-like mechanical properties but also high ionic conductivities. Therefore, OIPCs have been studied as solid electrolytes. However, the high ionic conductivity in the crystalline matrix is hard to understand because of large viscosity of solid phases. Several ion transports models have been suggested to understand its high ionic conductivity. Among them, experimental studies revealed the relation between ion conductivities and the volume of defects. Two kinds of defects were considered: point vacancies in crystalline phases and grain boundaries. However, the length and lifetime scales of point vacancies or grain boundaries are too short to investigate experimentally at the molecular level. In this talk, we conduct atomistic molecular dynamics simulation study of 1,3-dimethylimidazolium hexafluorophosphate ([MMIM][PF_6]) with four Li^+ ions as dopants. First, we propose the novel method to simulate the grain boundary structures in OIPCs. Radial distribution functions show that center parts of grains keep their original structure while boundary parts show broken and relatively disordered structures. Then, we compare the effect of point vacancies concentrations and the direction of grain boundaries on ion dynamics. With increasing point vacancies concentrations, all kinds of ions in [MMIM][PF_6] becomes more diffusive. However, at the boundaries, Li^+ ions in (100) show faster diffusion but cations in (100) show slowest diffusion among three grain boundary structures.

Poster Presentation : **PHYS.P-96**

Physical Chemistry

Event Hall THU 11:00~13:00

Thermodynamics and Kinetics of Multivalent Protein Interactions

Changeun Kim, Hyoin Park[1], Yongwon Jung[1], Jeong-Mo Choi*

Department of Chemistry, Pusan National University, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

A multivalent interaction refers to an interaction between two molecules having multiple conjugate modules that can form physical bonds, and it can be used to obtain stronger bonds by collecting weak monovalent interactions. The intermolecular and intramolecular interactions determine the thermodynamics and kinetics of multivalent interactions. Theoretical discussion has been mostly limited to the thermodynamic aspect, as the kinetic data were challenging to obtain experimentally. In this study, we studied the multivalent interactions between several types of protein pairs, by observing the kinetics of association and dissociation through surface plasmon resonance (SPR). The thermodynamic and kinetic data, i.e., rate constants (k_on and k_off) and equilibrium constant (K_D), could be used to analyze the nature of intermolecular and intramolecular interactions between multivalent proteins. As a result, it was shown that the thermodynamics of intramolecular interactions depends on the topology and valence of multivalent proteins. Deeper understanding of the physicochemical basis of multivalent interactions will help us design and engineering of biomolecular processes that involve multivalent interactions, such as biomolecular phase separation and drug design.

Poster Presentation : **PHYS.P-97**

Physical Chemistry

Event Hall THU 11:00~13:00

Theoretical Investigation of Optical Properties of six DTPs

Seongjae Lee, Dakyeung Oh, Joonghan Kim*

Department of Chemistry, The Catholic University of Korea, Korea

We performed density functional theory (DFT) and time-dependent DFT (TDDFT) calculations for the ground and excited states of of six DTPs such as P-Phenyldithieno[2,3-b:3’,2’-f]phosphepine (1α), P-Phenyldithieno[3,2-b:2’,3’-f]phosphepine (1β), P-Phenyldithieno[2,3-b:3’,2’-f]phosphepine-P-oxide (5α), P-Phenyldithieno[3,2-b:2’,3’-f]phosphepine-P-oxide (5β), 2,2’-Bis(phenylethynyl)-P-phenyldithieno[2,3-b:3’,2’-f]phosphepine-P-oxide (6α), 2,2’-Bis(phenylethynyl)-P-phenyldithieno[3,2-b:2’,3’-f]phosphepine-P-oxide (6β)). Coupled-cluster singles and doubles with perturbative triples (CCSD(T)) and multi-state complete active space second-order perturbation theory (MS-CASPT2) calculations are also performed to compare the results with those of DFT and TDDFT. The absorption and emission characters of six DTPs are analyzed using molecular orbitals and natural transition orbital analysis. The effect of S position on the electronic properties is also discussed.

Poster Presentation : **PHYS.P-98**

Physical Chemistry

Event Hall THU 11:00~13:00

Effect of Polymer Network Structure on Heterogeneous Diffusion Dynamics of Single Probe Molecules

Hyeyoung Joung, Dongho Kang, Jaesung Yang[1,*]

Department of Chemistry, Yonsei University, Korea
[1]*Department of Chemistry and Medical Chemistry, Yonsei University (Wonju), Korea*

The structural nature of polymer network in crowded environments, such as polymer melt, solution, and solvent-swollen thin film, is one of the primary factors affecting system’s physical properties, such as viscoelasticity, permeability, brittleness, tensile strength, mass transport property, and plasticization process, and may be significantly altered by modulating constituent single chain conformation. In this poster, we show the comparison of structural heterogeneity of inter- and intra-chain entangled polymer networks in solvent-swollen films of poly(methyl methacrylate) (PMMA), by applying solvent vapor swelling (SVS) and single particle tracking (SPT) techniques. Thin films composed of each type of network were prepared by an exquisite choice of processing solvent based on the Flory-Huggins theory and following systematic swelling of films, the diffusion of fluorescent probe N,N’-dipentyl-3,4,9,10-perylenedicarboximide (PDI) was tracked by recording videos. We managed to develop a custom computer program written in Python and assessed single-molecule trajectory, mean squared displacement, van Hove correlation function, and non-Gaussian parameter. We show that the mobility of PDI increases with degree of film swelling in both types of PMMA networks, however, the poor solvent-derived intra-chain entangled network is generally more heterogeneous in network structure, causing a previously unreported additional long-distance hopping. This work demonstrates that the structural nature of polymer networks has a dominant influence on the mass transport in soft matter systems.

Poster Presentation : **PHYS.P-99**
Physical Chemistry
Event Hall THU 11:00~13:00

Spectroscopic Studies of O_2 activation by an Organonickel Complex

Suyeon Gwon, Wooyeol Ryu, Jiseon Lee, Kiyoung Park*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Transition metal-mediated activation of dioxygen is important for the studies of oxygenation catalysts and metalloenzymes in nature. Previous studies on O_2 activation have mainly focused on copper and iron complexes because those are prevalent in O_2-activating enzymes. Alternatively, aerobic nickel-based oxidation chemistry in nature is limited to few enzymes.[1] Thus, nickel-O_2 chemistry is generally less developed than for most other 3d transition metals. In the previous study of O_2 activation by nickel, electron-rich ligands or other electron sources were used to reduce O_2. Recently, we have found that an organonickel complex, $(bpy)Ni^{II}(CH_2CMe_2\text{-}o\text{-}C_6H_4)$, can activate O_2 in an inner-sphere manner as forming oxygenated intermediates. By determining reaction kinetics, we have isolated a key intermediate and characterized its electronic and geometric structures by employing various spectroscopic techniques such as nuclear magnetic resonance, electronic absorption, and resonance Raman spectroscopy. The binuclear high-valent dinickel intermediate defined thus reveals that the organonickel complex can activate O_2 fully to the oxo level without exogenous electron sources.

1) Boer, J. L.; Mulrooney, S. B.; Hausinger, R. P.; Nickel-dependent metalloenzymes. *Arch. Biochem. Biophys*. **2014**, *544*, 142-152

Poster Presentation : **PHYS.P-100**

Physical Chemistry

Event Hall THU 11:00~13:00

Binding site prediction from sequence through graph convolutional network

Dongwoo Kim, Juyong Lee[1,*]

Lab of computational biology and chemistry, Kangwon National University, Korea

[1]*Department of Chemistry, Kangwon National University, Korea*

Disease-causing proteins are still being discovered, and most of them do not even know where the inhibitor will interact with the protein. When designing a drug, one of the most important considerations is where the inhibitor binds to the target protein.In this study, We have developed a new structure-aware method to predict the residues that consist of binding sites by using a graph convolutional network (GCN).We obtained node features from the structural characteristics of protein residues, such as secondary structure, phi/psi angles. The residue-pair type and their pairwise distance are used as the edge features of GCN.This approach is expected to have a better effect than the existing tree-based binding site prediction machine learning.Our model could be easily extended to other protein prediction tasks requiring a raw protein sequence.We further believe that this study will help design drugs.

Poster Presentation : **PHYS.P-101**

Physical Chemistry

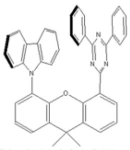
Event Hall THU 11:00~13:00

Theoretical study on tadf emitters of Donor-Bridge-Acceptor type

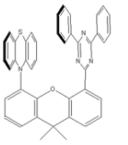
Jihyun Moon, Dongwook Kim*

Department of Chemistry, Kyonggi University, Korea

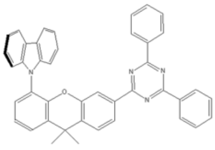
Thermally Activated Delayed Fluorescence (TADF) is considered an alternative to phosphorescence for organic light emitting diode (OLED) applications. The TADF phenomenon allows highly efficient emission by the up-conversion of triplet excitons to singlet excitons through the Reverse Intersystem Crossing (RISC) process. Thus, a device with up to 100% internal quantum efficiency can be manufactured. In this study, we deal with TADF emitters having an Electron Donor-Bridge-Electron Acceptor structure. Phenothiazine and carbazole are two different donor groups; 9,9-dimethylxanthene and diphenyltriazine are bridge and acceptor units, respectively. The second-order algebraic diagrammatic construction (ADC(2)) and density functional theory (DFT) methodologies are used for the electronic structure calculations. By conducting various analyses, such as natural transition orbitals, excitation energy decompositions, etc., we investigate the effect of molecular topology on the factors associated with RISC process in TADF emitters.



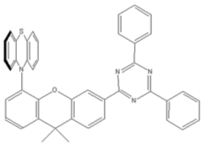
9,9-dimethyl-4-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-9*H*-carbazole



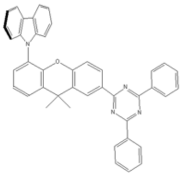
10-(9,9-dimethyl-4-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-10*H*-phenothiazine



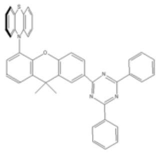
-(9,9-dimethyl-3-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-9*H*-carbazole



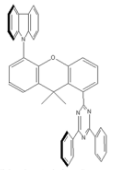
10-(9,9-dimethyl-3-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-10*H*-phenothiazine



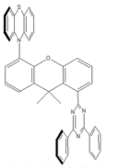
9-(9,9-dimethyl-2-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-9*H*-carbazole



10-(9,9-dimethyl-2-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-10*H*-phenothiazine



9-(9,9-dimethyl-1-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-9*H*-carbazole



10-(9,9-dimethyl-1-(4,6-diphenyl-1,3,5-triazin-2-yl)-9*H*-xanthen-5-yl)-10*H*-phenothiazine

Poster Presentation : **PHYS.P-102**

Physical Chemistry

Event Hall THU 11:00~13:00

The dynamics of bimolecular proton transfer in aqueous solution using Time-resolved Infrared spectroscopy

JuHyang Shin, Manho Lim*

Department of Chemistry, Pusan National University, Korea

The neutralization of an acid by a base is one of the fundamental reactions in solutions. We observed aqueous bimolecular proton transfer, using a photoacid, 8-hydroxy-1,3,6-trisulfonate-pyrene (Pyranine, PyOH), which reacts with azide (N_3^-) as a strong acid when electronically excited. The most significant IR spectra changes of PyOD between electronic ground-state and excited-state occur in the spectral region of 1400-1650 cm^{-1}. Azide has a strong band at 2042 cm^{-1} and its conjugated acid (DN_3) at 2133 cm^{-1}. Time-resolved vibrational spectra were measured in these spectral regions after excitation of PyOH in the presence of N_3^- in D_2O solution with a 400-nm pulse. In the presence of low base concentration (< 150 mM of N_3^-), the dominant reaction path was found to be the bimolecular reaction between the base molecule and deuteron (D^+) which was dissociated from the excited state PyOD, rather than direct reaction from acid-base complexes that was observed in high base concentration. The bimolecular reaction involved in acid-base reaction observed via this research will be presented.

Poster Presentation : **PHYS.P-103**

Physical Chemistry

Event Hall THU 11:00~13:00

Development of a capillary-based SERS sensor for Galactose detection

Eun Hae Heo, Hyejin Chang*

Division of science education, Kangwon National University, Korea

Galactosemia is a inherited metabolic disorders in which galactose accumulates in the body by disrupting the normal metabolism of galactose due to enzyme deficiency. Therefore, development of a ultrasensitive, selective and reliable approach to detect galactose is important for a proper treatment. In this presentation, we report a surface-enhanced Raman scattering (SERS) sensor using capillaries for easy detection of galactose. The developed SERS sensor was developed by decorating the inner wall of capillary with silver nanoshells (AgNSs) and using 4-mercaptophenylboronic acid (4-MPBA) as a label compound. In our experimental design, oxidation of galactose by a galactose oxidase (GOx) enzyme converts 4-MPBA to 4-mercaptophenol (4-MPhOH), leading to the formation of H_2O_2. Our sensor showed high selectivity and sensitivity. These results indicated that these capillary sensors had great potential for galactose detection for diagnosis. Details of the results will be discussed in the presentation.

Poster Presentation : **PHYS.P-104**

Physical Chemistry

Event Hall THU 11:00~13:00

Fabrication of Laser Scanning Confocal Fluorescence Microscope System for Single Particle Spectroscopy

Jaesang Yu, **Jaesung Yang**[1,*]

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Single-particle fluorescence spectroscopy has proven very valuable for the investigation of various functional nanomaterials. Especially, halide perovskite nanocrystals considered as promising materials for a wide range of applications such as solar cells, light-emitting devices, and lasers have been extensively studied at the single particle level for a deeper understanding of the charge carrier dynamics, with the ultimate goal of enhancing the solar cell efficiency hopefully beyond the Shockley-Queisser limit. In this poster, we show the fabrication of a custom-built laser scanning confocal fluorescence microscope system, with which we intend to investigate photophysical and optical properties of perovskite quantum dots (QDs) and conjugated polymer aggregates on an individual basis. The system is based on an inverted type optical microscope coupled to a picosecond pulsed diode laser. The two-dimensional raster scan is achieved by using a galvanometer scanner. Fluorescence emission from single molecules is divided by beam splitters and focused onto a photomultiplier tube (PMT), an avalanche photodiode (APD) coupled to a TCSPC card, and an EMCCD through a spectrograph to obtain raster-scanned image, fluorescence intensity trajectory and time-resolved decay profile, and photoluminescence spectrum, respectively. We show preliminary data obtained using commercially available semiconductor QDs (CdSeS/ZnS QDs) and lead halide perovskite QDs ($CsPbBr_3$) synthesized by the hot-injection method.

Poster Presentation : **PHYS.P-105**

Physical Chemistry

Event Hall THU 11:00~13:00

Binding affinity prediction using graph convolution network

Jaemin Sim, Juyong Lee*

Department of Chemistry, Kangwon National University, Korea

Predicting the protein-ligand binding affinity is an important step for drug screening and discovery. Various machine-learning or deep-learning methods have been proposed to predict the poses of protein-ligand complexes and to better predict binding affinity. In this study, we propose a new protein-ligand binding affinity prediction model based on the graph convolution network (GCN). To create such a GCN model, protein-ligand binding affinity is predicted using data from the protein's pocket in the pdbbind data set. The model is devised by representing the atoms of protein and ligands as the nodes and spatially adjacent atoms are considered connected. The model generated in this way is trained using the PDBbind general set, and evaluated by comparing it with actual binding affinity with data from the casf-2016 set. The results show that our GCN-based model shows better or comparable accuracy to existing DL-based models.

Poster Presentation : **PHYS.P-106**

Physical Chemistry

Event Hall THU 11:00~13:00

Synthesis and Photophysical Properties of Remarkably Luminescent Cesium Lead Bromide Perovskite Quantum Dots

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In the past few decades, $CsPbX_3$ (X = Cl, Br, and I) perovskite quantum dots (PQDs) have emerged as promising material for applications in next-generation optoelectronic devices due to their surpassing photophysical properties such as bandgap tunability, long-range mobility of charge carriers, and high photoluminescence (PL) quantum yield (QY). Because of these advantages, PQDs have been the subject of active research in the development of optoelectronic devices such as solar cells, light emitting diodes, and lasers. To optimize their functionality in the devices, it is necessary to understand the fundamental properties of these types of materials. In this poster, we show the synthesis and photophysical properties of a couple of $CsPbBr_3$ PQDs. The powder X-ray diffraction (PXRD) and transmission electron microscope (TEM) measurements reveal that the crystal structure of the synthesized $CsPbBr_3$ PQDs have the orthorhombic phase and the average size varies between 9-12 nm in diameter. Optical absorption and emission spectra were also measured. The emission peaks of the $CsPbBr_3$ PQDs dispersed in toluene are located at 500-515 nm, with the peak becoming red-shifted as the size increases. They show strong PL intensity, narrow full width at half maximum (FWHM) of 16-20 nm, and high QY of 70-80%. While the observed values of QY are already sufficiently high, it is widely known that PQDs typically suffer from fluorescence quenching due to the local charge trapping and concomitant non-radiative recombination process. To further improve fluorescence properties, we attempted to synthesize tri-n-octylphosphine (TOP)-$CsPbBr_3$ QDs, where TOP assures a more robust surface passivation. As a result, we could achieve very high QY, reaching up to about 92%. The PQDs shown here will be subject to single particle spectroscopy using a laser scanning confocal fluorescence microscope our group has very recently fabricated.

Poster Presentation : **PHYS.P-107**

Physical Chemistry

Event Hall THU 11:00~13:00

Interplay among locally excited, charge-transfer, and charge-separated states in a donor–acceptor copolymer single chain

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Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Organic photovoltaics (OPVs) have been extensively highlighted as promising photovoltaics for realizing low-cost solar energy conversion with light weight and applicability for flexible devices. With introducing non-fullerene acceptors, the performance of bulk-heterojunction OPV devices has significantly improved, reaching the power-conversion efficiency (PCE) higher than 18%. In this work, we revealed the photoinduced dynamics in a single chain of donor–acceptor (D-A) polymer, PM6, which has been widely used as a donor in the state-of-the-art non-fullerene OPV systems with its top-notch PCE performance[1]. With the femtosecond-resolved absorption and fluorescence spectroscopy spanning sub-ps to μs time domains, we explored the evolution of locally excited (LE), charge-transfer (CT), charge-separated (CS) states in the single chain of PM6[2]. Our observation revealed that an intrachain CT state forms within 200 fs and establishes an ultrafast equilibrium with the parent LE state. We tracked the dependence of the evolution of these equilibrated states on the length of the chain. The equilibrated LE and intrachain CT states persist until they diffuse and reach a chain folding. At the chain folding, the intrachain CT state quickly transforms into an interchain CT state that bifurcates into forming a CS state or annihilation within a picosecond. Our findings highlight the role of chain foldings for maximizing polaron generation in OPVs based on PM6.References[1] B. Lee, S. Kim, H.-W. Nho, J. Oh, G. Park, M. Jeong, Y. Cho, S. M. Lee, O.-H. Kwon, and C. Yang, *Adv. Energy Mater.*, 2021, **11**, 2102594.[2] H.-W. Nho, W.-W. Park, B. Lee, S. Kim, C. Yang, O.-H. Kwon, *Phys. Chem. Chem. Phys.*, 2022, **24**, 1982–1992.

Poster Presentation : **PHYS.P-108**

Physical Chemistry

Event Hall THU 11:00~13:00

Excited-state proton transfer of a cationic photoacid in a nanoscopic water pool

Hak-won Nho, Oh-Hoon Kwon*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Reverse micellar (RM) structure has been extensively studied as prototypes mimicking water pockets in biological machinery. The RM system consists of three distinct phases: a hydrophobic phase outside, a water pool confined inside, and an interfacing headgroup region. The confined water molecules are usually referred to as two structurally and dynamically distinct portions. The highly constrained “bound” water is clearly distinguishable from the bulk-like “free” water residing in the water pool core. The hydrophilic RM interface strongly traps the bound water molecules. Therefore, the bound water molecules are highly viscous and the hydrogen-bonding network near the RM interface is rigid then free water. This structural feature induces a heterogenic environment with dielectric and viscosity gradients in the confined water pool.We chose an anionic RM interface and a unique prototropic probe, *N*-methyl-7-hydroxyquinolinium in the AOT RM to investigate how hydration dynamics and the excited-state proton-transfer (ESPT) reaction of the prototropic cationic probe responds to the confined heterogenous environment [1-3]. The cationic probe tightly binds to the anionic RM interface. From the analyses of population dynamics, the interface-bound probe was found to sense the wide range of the water molecules, which reside in not only the bound water layer, but also the free core water. In this study, we revealed how the ESPT dynamics of the probe responds to the gradient of the heterogenous environment in confined water pool on the several picoseconds to nanosecond timescales. We suggest also the ESPT-assisted migration of the probe because the probe loses its cationic charge during the ESPT. The solvation correlation function, v(t), and intensity profiles, I(t), from the deconvolution of time-resolved fluorescence spectra were the key observables for understanding the chemical reaction dynamics and motion of the probe within the confined water pool.Reference[1]A. Adhikari, J.-H. Park, H.-W. Nho and O.-H. Kwon, J. Mol. Liq. 2020, 320, 114346.[2]H.-W. Nho, J.-H. Park, A. Adhikari and O.-H. Kwon, J. Mol. Liq. 2021, 326, 115270.[3]H.-W. Nho, A. Adhikari and O.-H. Kwon, J. Phys. Chem. B., in press.

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Poster Presentation : **PHYS.P-109**

Physical Chemistry

Event Hall THU 11:00~13:00

Ultrafast spectroscopic investigation on the photoluminescence of carbon nanodots

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Carbon-based materials such as carbon nanodots, graphene, and carbon nanotubes are currently receiving attention because of their remarkable properties and great potential for a variety of applications. Among them, carbon nanodots (CND) can be used for bio-images, photocatalysis, and optical sensing due to their high luminescence yield, but it has not yet been revealed what the origin of the luminescence is.[1] In this study, we synthesize CND using microwave oven and conduct time domain spectroscopies such as time-correlated single photon counting (TCSPC), time-resolved fluorescence by frequency up-conversion, and transient absorption (TA) for finding out what the origin is. From the time-resolved fluorescence spectrum (TRES), the change of the isoemissive point was observed according to the concentration with the picosecond time scale. Also, the observation of nuclear wavepacket oscillation was attempted and observed a clear oscillation at 627 cm^{-1} from TA experiment. From the ultrafast spectroscopic investigation on the photoluminescence of carbon nanodots, it was confirmed that there are two luminophores emitting luminescence in CND, and in the case of redshifted luminophore, it have a motion related to 627 cm^{-1}. We speculate that the luminophore is a kind of benzinoid structure molecules, and try to clarify what it is.**References**[1] Das, S.K.; Liu.Y; Yeom. S; Kim, D. Y.; Richards, C.I., *Nano Lett*., **2014**, *14*, 620.

Poster Presentation : **PHYS.P-110**

Physical Chemistry

Event Hall THU 11:00~13:00

A Comprehensive Investigation of Electron Push-Pull Effect on Both Neutral and Radical Species of the Perylene-Based D−π−A System

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To investigate the substituent effects on both neutral and radical species, the donor−π−acceptor (**D−π−A**) structure compound using perylene as a π-bridge was designed and synthesized by having the same acceptor (2,4-diphenyl-1,3,5-triazine (TRZ)) and modifying only the donor (diphenylamine (DPA)) substituent. The photophysical and electrochemical properties of the neutral species **DPA(R)−Peri−TRZ** (R=F, H, Me, and OMe) were investigated, and predictable ICT properties were observed based on previous studies. Using the fact that ICT can be controlled according to the substituents, the effect of substituents on radical species was proposed and the supporting evidence was confirmed through spectroelectrochemical (SEC) studies. SEC studies were performed based on electrochemical data and both radical anionic and cationic species from redox active acceptor and donor were observed. The anionic species generated from acceptor (TRZ) in SEC shows no significant change according to the substituent, but the cationic species generated from the DPA donor had an increase in Δ absorbance from electron-withdrawing group to -donating group. The effect of controlling the substituents for both neutral and radical species was verified not only experimentally but also theoretically, and the trends of both experimental and theoretical data were consistent. Currently, our group is conducting research on radical substances as an extension of this study, and it is expected that controllable radical substances will be diversified through this research.

Poster Presentation : **PHYS.P-111**

Physical Chemistry

Event Hall THU 11:00~13:00

Development of a dual SERS substrate using graphene quantum dot and silver nanoshell

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Since Raman enhancement of graphene has been reported, a dual enhancement platform, which uses both metal nanostructures based plasmonic signal enhancement and graphene based chemical enhancement (CM) has drawn attention for overcoming limitation of conventional Surface-Enhanced Raman Scattering (SERS). Dual enhancement system guides analyte molecules with low surface affinity for plasmonic nanoparticles close to the metal surface to increase electromagnetic enhancement (EM) and simultaneously CM by graphene can also be used. In this study, a substrate using graphene quantum dots (GQDs) and bumpy Ag nanoshells (AgNSs) on a solid support was designed to develop a dual SERS system. To observe dual-enhancement at single particle level, we fabricated a hydrophobicity-controlled self-assembled monolayer on a silicon wafer and used selective interactions among the silicon wafer, AgNS and GQDs. The fabricated SERS substrate was characterized by SEM, EDS, AFM, and Raman spectroscopic analysis. Using rhodamin6G and malachite green as probe molecules, the Raman enhancement effect of CM on GQDs could be quantified in our dual SERS system.

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Poster Presentation : **PHYS.P-112**

Physical Chemistry

Event Hall THU 11:00~13:00

Simultaneous Deposition of Amorphous NiFeOx and Co-Pi on the Surface of Hematite (a-Fe2O3) Photoanode: Dependence on the Order of Arrangement of the Treatments

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We prepared hematite (a-Fe2O3)-based photoanode, simultaneously treated by an amorphous NiFeOx coating and a cobalt-phosphate catalyst (Co-Pi), and investigated the dependence of the photoelectrochemical (PEC) performance on the order of arrangement of the treatments. We found that the PEC performance of the film in which Co-Pi was deposited on the surface of hematite first, followed by the NiFeOx coating, was higher than that of the sample where the order of the treatments was reversed. We will discuss the origin of the effect of the treatments on the PEC performance, based on the results obtained by various spectroscopic techniques.

Poster Presentation : **PHYS.P-113**

Physical Chemistry

Event Hall THU 11:00~13:00

Selectivity of Method for Zinc-Amino Acid Complex Through Quantum Calculation

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Metal-amino acid complexes are useful substances for the body and are studied not only in the nutritional field, but also because of their anticancer, antibacterial, and catalytic actions in the body of metal compounds. Density functional theory (DFT) is useful for predicting the properties of metal-amino acid complexes through quantum calculations. However, the conventional calculation method does not properly represent the properties of the metal-amino acid complex generally constituting the polymer. Therefore, calculations were performed taking the intermolecular polymerization form into consideration. In addition, IR spectral analysis was added to the comparison of intra-atomic distances to quantify the calculation results of various methods.

Poster Presentation : **PHYS.P-114**

Physical Chemistry

Event Hall THU 11:00~13:00

Estimation Binding Affinity of domain-domain interaction with coarse-grained systems

Jinyoung Byun, Juyong Lee*

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We investigated the protein-protein interactions between the domains of amyloid precursor protein (APP) using coarse-grained models using the Martini force field version3. We used the initial ternary complexes (E1-E1, E2-E2, E1-KPI, E2-KPI, and KPI-KPI) generated by both HaDDock and AlphaFold2, which are one of the state-of-art modeling methods. By using the Umbrella sampling method, we estimated the binding affinities of each system similar to experimental results. Our results show that E1-KPI and KPI-KPI domains have attractive interactions while the other domains do not interact significantly. This result explains why APP751 proteins interact with each other, while APP695 proteins do not.

Poster Presentation : **PHYS.P-115**

Physical Chemistry

Event Hall THU 11:00~13:00

Spectroscopic and Computational Studies of Ligand-field Excitation-induced C-S Bond Formation from Nickelacycles

<u>Jiseon Lee</u>, Jeongcheol Shin, Kiyoung Park[*]

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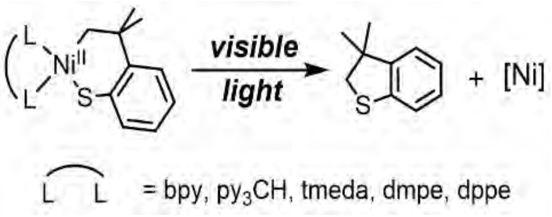
In conventional Ni-catalyzed cross-coupling reactions such as Negishi, Suzuki, and Kumada reactions, bond-forming reductive elimination (RE) reactions of Ni(II) complexes require high-temperature conditions or extended reaction time. The rate-determining RE reactions of organonickel(II) species can be facilitated by inducing electronic excitation via energy transfer from photocatalysts or direct photoexcitation. Despite increasing examples of excited-state Ni chemistry, no consensus has been yet established for detailed mechanisms of organonickel(II) photoreactions. We have investigated the excited-state C-C, C-O, and C-S bond-forming RE activities of nickelacycles with cycloneophyl ($-C_6H_4\text{-}o\text{-}C(CH_3)_2CH_2\text{-}$) and its oxa- ($-OC_6H_4\text{-}o\text{-}C(CH_3)_2CH_2\text{-}$) and thia- ($-SC_6H_4\text{-}o\text{-}C(CH_3)_2CH_2\text{-}$) derivative ligands.[1] Among 17 species studied with five different ancillary ligands, only C-S bond formation could be achieved in an excitation-energy-dependent manner. To understand this excited-state RE activity, the electronic structures of nickelacycles have been characterized by utilizing electronic absorption and magnetic circular dichroism spectroscopies and density functional theory computations. The analysis results have revealed that the Ni-C bond homolysis of nickelacycles can be induced by ligand-field excitations resulting Ni(I) intermediates regardless of the ancillary ligands.

[1] J. Shin, J. Lee, J.-M. Suh, K. Park. *Chem Sci.*, **2021**, *12*, 15908-15915



Poster Presentation : **PHYS.P-116**

Physical Chemistry

Event Hall THU 11:00~13:00

Nonlinear pulse compression down to 15 fs at near-infrared range using photonic crystal fiber and its application to time-resolved spectroscopy

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Femtosecond pulse generation technique and its application to time-resolved spectroscopy lead to further understanding of fundamental processes in chemistry. For example, observing vibrational coherences, such as nuclear wave packet (NWP), in a system can gives information about structural changes related to the process. To measure the rapid changes of the system, the higher time-resolution of measurement is needed.

Here we performed short pulse generation at near-infrared range using nonlinear pulse compression using photonic crystal fiber (PCF). The 1200 nm pulses with 59 fs duration, seeded by cavity-dumped optical parametric oscillator[1], were injected into PCF and spectrally broaden mainly by self-phase modulation. The output pulses from the PCF were GVD compensated and it was compressed down to 15 fs. The autocorrelation traces of the nonlinear compressed pulses are not ideal-Gaussian, consists of main peak and surrounding shoulders. By frequency doubling of the compressed 1200 nm pulses, we obtained 600 nm pulses with 13 fs duration and removed shoulders. The main peaks of compensated 600/1200 nm pulses were nearly the same with the transform limited pulses in the autocorrelation traces.

To demonstrate the applicability of nonlinear pulse compression to the time-resolved spectroscopy, the newly generated pulses by the nonlinear pulse compression were applied to time-resolved fluorescence(TF) measurement – 600 nm and 1200 nm pulses were used as pump and probe, respectively. The instrumental response function (IRF) of the TF measurement had FWHM of 21 fs, which can be expected to resolve rapid changes up to ~1100 cm^{-1}. The IRF also had some artifacts around the main peak, but its intensity was limited to that not exceeding 20% of the main peak.

References

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Poster Presentation : **PHYS.P-117**

Physical Chemistry

Event Hall THU 11:00~13:00

Role of electrostatic interactions in phase separation of gephyrin

Da-Eun Hwang, Jeong-Mo Choi[*]

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Liquid-liquid phase separation (LLPS) of biomolecules has recently attracted broad interest due to its role in the spatiotemporal compartmentalization of eukaryotic cells. Postsynaptic density (PSD) is a cellular condensate composed of hundreds of proteins, colocalized with the postsynaptic membrane of excitatory synapses. It was shown that various scaffolding proteins in excitatory synapses form PSD through LLPS, and among them, gephyrin is the core scaffolding protein in inhibitory PSDs. Gephyrin consists of two folded domains (N-terminal G domain and C-terminal E domain) and a large unstructured linker that connects the two. Recently, the mechanism of gephyrin clustering in PSDs through liquid-liquid phase separation was experimentally elucidated. However, the molecular mechanism behind this collective behavior is yet unclear. We used atomistic Monte Carlo simulations of the wild-type and mutant systems to obtain molecular insights and found that the electrostatic interactions between the basic residues on the disordered linker and the acidic residues on the E domain are critical in determining the structural ensemble. We hypothesize that the same electrostatic interactions are the driving force of gephyrin LLPS, which leads to the prediction that perturbation of the key residues will decrease the LLPS propensity.

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Poster Presentation : **PHYS.P-118**

Physical Chemistry

Event Hall THU 11:00~13:00

Origami structure-based flexible crystalline silicon substrate

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Flexible solar cells are spotlighted as next-generation solar cells because they can be installed on uneven and movable surfaces. Among them, flexible crystalline silicon (c-Si) solar cells show relatively high efficiency and stability rather than other solar cells. However, flexible c-Si solar cells exhibit poor light absorption properties by their thin c-Si substrate. In this study, we present a novel strategy that can show flexible properties on thick c-Si wafers. This strategy is to achieve flexible property of thick c-Si wafers by employing an origami structure on the c-Si wafers. The origami structure could be flexible thanks to a spring shape configuration. As a result, the origami structure-based thick (~ 525 um) c-Si wafer shows outstanding flexibility compared to bare c-Si wafer. When the fabricated c-Si substrate is applied as a flexible photovoltaic device, we expect that inherent low light absorption property of thin c-Si photovoltaics can be thoroughly overcome.

Poster Presentation : **PHYS.P-119**

Physical Chemistry

Event Hall THU 11:00~13:00

Computational Redox Potentials Relevant to Bioinorganic Chemistry

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From the development of computers and theories, quantum chemical molecular modeling is being used as a powerful tool in understanding chemical reactions. Computing redox potential is also an excellent field to utilize. With inexpensive density functional theory methods, prediction on the change of molecules after the redox events is possible. However, due to the gap between the experimental condition and computational methods, the calculated potentials may not match the experimental ones. Irreversible potential or ion-pairing effects could be the cause of these errors. Herein, we give a tutorial on computing redox potentials and provide a benchmark assaying efficient and widely available methods. Also, potential pitfalls and how to avoid them are discussed.

Poster Presentation : **PHYS.P-120**

Physical Chemistry

Event Hall THU 11:00~13:00

Spectroscopic and computational studies on O_2 reaction of a mononuclear Co(II) complex

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Dioxygen is an eco-friendly, economical, and strong oxidant, but activating O_2 by divalent Co(II) species is thermodynamically challenging because of its relatively high effective nuclear charge. In collaboration with Prof. Mi Hee Lim's group at KAIST and Prof. Jaeheung Cho's group at UNIST, we have discovered that a Co(II) complex with the macrocyclic tetradentate N4 ligand, *N*,*N*'-di-tert-butyl-2,11-diaza[3.3](2,6)pyridinophane (TBDAP, Figure 1) can react with O_2 in aqueous media, displaying a long time-scale reaction (>100 hours) with significant variations in electronic absorption and magnetic circular dichroism spectra. The intermediates and product of the reaction have been characterized with ESI-MS, NMR, and resonance Raman, IR spectroscopies, and their structural candidates have been assessed with density functional theory computations that reproduce electronic and vibrational spectroscopic features. These analyses have shown that the O_2 reaction in aqueous media can result in *N*-dealkylation of the TBDAP ligand via C-H bond activation of reactive oxygen species. This study has revealed that aqueous media can promote O_2 activation by amplifying ROS species.

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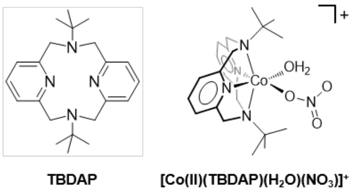

TBDAP

$[Co(II)(TBDAP)(H_2O)(NO_3)]^+$

Figure 1. Chemical structures of the TBDAP and $[Co(II)(TBDAP)(H_2O)(NO_3)]^+$.

Poster Presentation : **PHYS.P-121**

Physical Chemistry

Event Hall THU 11:00~13:00

Studying Unusual Molecular Aggregation of Quinocyanine in the Charged Droplets

Sanghwang Park, Jongcheol Seo*

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Charged droplets can be easily observed in the field of mass spectrometry. In charged droplets generated by electrospray ionization (ESI), a method of converting a solution sample into gaseous ions, unique molecular behaviors different from those in bulk solution appear. Formation of unusual molecular aggregates is an example of the interesting molecular behaviors in the charged droplets. In this study, we investigated quinocyanine which exhibits the unusual aggregation in the charged droplets. Quinocyanine halide, which is well known to form J-aggregate in bulk solution, showed unique stacking behavior according to the ion mobility-mass spectrometry (IM-MS) results obtained through ESI. In positive mode, quinocyanine aggregates only with I-, even if other halides (Cl-, Br-) are present. On the other hand, there is a tendency to form aggregates with smaller halides in negative mode. These are unusual results that differ from the bulk solution. Our results are unusual results that differ from bulk solution and suggests that the halide selectivity of quinocyanine aggregates depends on the charge state. In future, X-ray scattering and fluorescence spectroscopy will be used for monitoring the unique stacking behavior of quinocyanine in the charged droplets. We expect that this research can solve the challenging and novel molecular aggregation in the charged droplets.

Poster Presentation : **PHYS.P-122**

Physical Chemistry

Event Hall THU 11:00~13:00

Effects of Phase Separation on Synthetic Genetic Circuits

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[1]*Department of Chemistry, Pusan National University, Korea*

Biomolecular phase separation in cells has been attracting attention from the related fields. Compartmentalization of gene products via phase separation was suggested to play an important role in reducing the biological noises. Some liquid compartments could maintain constant protein levels and lower the range of fluctuations. We examined the effects of phase separation on noises in the synthetic genetic circuits through simulations. The tested genetic circuits include the negative autoregulation circuit, the Goodwin model, and the repressilator. We numerically monitored the changes over time using the continuous model (differential equations) and the stochastic model (Gillespie algorithm). We confirmed that the stochastic model showed a relatively irregular period and amplitude compared to the continuous model and found that introduction of phase separation resulted in significant changes in the dynamics of the stochastic model.

Poster Presentation : **PHYS.P-123**
Physical Chemistry
Event Hall THU 11:00~13:00

Liquid-Liquid Phase Separation and Gelation of Polymers: from the Perspective of Percolation

Da-Hyun Koo, Jeong-Mo Choi*

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Biomolecular phase separation plays an important role in formation and regulation of various biomolecular condensates in cells. Two types of proteins, namely linear multivalent proteins and intrinsically disordered proteins, are known to drive phase separation, and they can be described by the stickers-and-spacers framework. In previous work, the framework was successfully implemented in a graph-based simulation module, which uses the concept of percolation, and the effects of intra-cluster interactions and cooperativity were investigated. Here, we apply the same simulation module to two simple archetypal systems, homopolymer A_n and block copolymer A_nB_n, and investigate the determinants of the threshold concentrations of phase separation and gelation. We also estimated the dwell time of each polymer molecule in condensates, which determines the diffusion behaviors of the constituent polymers.

Poster Presentation : **PHYS.P-124**

Physical Chemistry

Event Hall THU 11:00~13:00

Photoexcitation dynamics of S-nitroso-mercaptoethanol probed by Time-resolved IR spectroscopy

Hojeong Yoon, Seongchul Park, Manho Lim*

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S-nitrosothiol (RSNO) is often used as a reference in nitric oxide (NO) donor studies. In addition to the photodissociation kinetics after 330 nm excitation of various water-soluble RSNO reported in previous studies, this study reports the link between the electronic structural information of the intermediates produced after excitation and quantum chemical calculations. We used time-resolved IR spectroscopy (TRIR) to obtain photoexcitation spectra of S-nitroso-mercaptoethanol (MceSNO) that can be compared with the calculated results, and report the orbital analysis and potential energy curve of the photoexcitation intermediate. The electronic transition corresponding to the 330 nm excitation of MceSNO was analyzed from the nonbonding orbital of n_S to the π^* antibonding orbital of NO through natural transition orbital (NTO) analysis. As a result, the electrons of S undergo charge transfer toward the NO molecule, and the ionic bond of the S-N bond becomes stronger and the bond length becomes shorter. In terms of structure, the dihedral angle of R-S-N-O is changed from 0° to 90° to minimize the repulsive force between the nonbonding p orbital of n_S and the π^* antibonding orbital of NO. It then loses energy and undergoes internal conversion to a lower electronic state, which is observed in TRIR. On the other hand, after excitation, some undergo a dissociation process with a lot of kinetic energy. Among the higher excited states, the transition state of the nonbonding orbital of n_S to the σ^* antibonding orbital of S-N crosses the charge transfer transition channel. Excited MceSNO with kinetic energy dissociates through a crossover state during the motion.

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Poster Presentation : **PHYS.P-125**

Physical Chemistry

Event Hall THU 11:00~13:00

A study on Gold Nanoparticles via Levitator Coupled with Spectroscopy Techniques for In Situ Reaction Monitoring

Juhyeon Park, Ahreum Min, Jiwon Kim, Myong Yong Choi[*]

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Levitation enables containerless processing of single levitated droplets. This can avoid complex effects that occur at the contact surfaces of materials, such as reaction vessels, and increase the sensitivity of spectral detection techniques such as Raman spectroscopy or Fourier transform infrared (FT-IR) spectroscopy. Here, we design a pressure-compatible process chamber and describe an in-situ multispectral analyzer equipped with various spectroscopic analyzers attached to the levitation unit. The process chamber was connected to a spectroscopic probe of high-sensitivity Raman, FT-IR, and UV-Vis spectrometer using fiber optics to observe the physical and chemical changes of the suspended particles in real-time. In addition, we observed the photoreduction of gold ions by a pulsed laser in the floating particles in real-time using this instrument. This shows that the newly developed instrument is very suitable for real-time confirmation of the physical and chemical reaction processes of substances.

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Poster Presentation : **PHYS.P-126**
Physical Chemistry
Event Hall THU 11:00~13:00

Rational design of ultra-thin CoFe-LDH nanostructure as a highly efficient electrocatalyst for overall water splitting in alkaline medium

Shreyanka Shankar Naik, Theerthagiri Jayaraman, Seung Jun Lee, Yiseul Yu[1], Myong Yong Choi[*]

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Developing a highly active, durable, and cost-effective bifunctional electrocatalysts are in huge demand towards the overall water splitting applications. Among the various electrocatalysts, layer double hydroxide (LDH) has been exceptional towards oxygen evolution reaction (OER). We made an attempt to synthesize two dimensional CoFe-LDH nanostructure employing pulsed laser ablation technique in aqueous medium containing carbonate (CO_3^{2-}) as an intermediate anion. During the exfoliation of LDH samples creates coordinatively unsaturated metals which improves the intrinsic electronic conductivity of the material and results effective towards water electrolyzer reactions. The atomic ratio of cobalt (Co) and iron (Fe) were controlled by the duration of ablation of metal targets. Formation of the materials and their chemical compositions were characterized using XRD, FESEM, HRTEM and XPS analyses. During the half-cell oxygen evolution reaction in alkaline medium, CoFe-LDH (6-6) showed highest activity with the lowest overpotential of 298 mV at 10 mA/cm^2. Similarly, the other half reaction towards hydrogen evolution has been higher in the case of CoFe-LDH (4-8) samples with the overpotential of 365 mV at 10 mA/cm^2. Finally, an alkali-electrolyzer conataining CoFe-LDH (4-8) as both the cathode and anode could achieve a voltage of 1.89 V at the current density of 10 mA/cm^2. Along with higher activity, samples also showed significant chemical and structural stability for long run cycles. Additionally, our findings demonstrate the promising electrocatalytic activity of LDHs for scale-up alkaline water splitting.

Poster Presentation : **PHYS.P-127**

Physical Chemistry

Event Hall THU 11:00~13:00

Structure of the 3-cyanoindole and Its Solvent Clusters in the Gas Phase: A Spectroscopic and Computational Study

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Department of Chemistry, Gyeongsang National University, Korea

The structural information of the excited states of 3-cyanoindole ammonia cluster, 3CI-$(NH_3)_1$, in molecular beams was investigated in the gas phase. We obtained UV-UV hole-burning spectrum (UV-UV HB) to determine the number of conformers present in the molecular beams and to examine their spectral features. As a result, single conformer of 3CI-$(NH_3)_1$ was observed in the mass- selected one-color resonant two-photon ionization (1C-R2PI). The origin band of 3CI-$(NH_3)_1$ in the R2PI spectrum is red-shifted by 122 and 71 cm^{-1} compared to those of the 3CI monomer and 3CI 1:1 water cluster, 3CI-$(H_2O)_1$, respectively. The fully optimized geometries, relative energies, transition energies, binding energies, and electrostatic potential (ESP) of the 3CI monomer, 3CI-$(H_2O)_1$ and 3CI- $(NH_3)_1$ clusters were calculated at the B3LYP and TD-B3LYP methods with the 6-311++(d,p) basis set. The observed spectra are compared with the predictions of time-dependent density functional theory (TD- DFT) calculations.

Poster Presentation : **PHYS.P-128**
Physical Chemistry
Event Hall THU 11:00~13:00

Photo-induced Intramolecular C-H bond Activation of a Mononuclear Non-Heme Oxoiron(IV) Complex

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Mononuclear non-heme oxoiron(IV) species are key intermediates in the catalytic cycles of various iron-dependent dioxygenases which can effectively induce C-H bond activation. [1],[2] To mimic the C-H bond activation activity of the enzymatic oxoiron(IV) intermediates, more than 80 mononuclear non-heme oxoiron(IV) complexes have been synthesized and further extended to the heterogeneous systems such as iron-based zeolite Socony Mobil-5. [3] The C-H bond activation is initiated as the oxoiron(IV) intermediates abstract hydrogen atoms from substrate. The DFT and ab initio calculated reaction coordinates of this process suggest that the oxoiron(IV) center converts to oxyliron(III) at the transition state to effect the radical transfer. [4] Moreover, another spectroscopic and computational study revealed that there is spin-crossover from S=1 to S=2 states in excited level. In this study, photoexcitation has been utilized to the S=1 oxoiron(IV) complex to induce the S=2 states, which is known to be reactive spin states in hydrogen atom transfer than S=1 states. [5] Upon irradiation of 355 nm light, [(TMC)Fe(IV)(O)(NCMe)]$^{2+}$ decays within an 1 hour to generate the precursor of the oxoiron(IV) complex, [(TMC)Fe(II)]$^{2+}$ and its hydroxylated derivative. Notably, this photochemical reaction from the oxoiron(IV) complex proceeded even at an extremely low temperature, indicating that photo-induced C-H bond activation is not limited by thermal energy. To understand the unique photo-reactivity of the oxoiron(IV) complex, various spectroscopic techniques have been employed. These analyses reveal that a strong C-H bond of the aliphatic ligand can be activated by the excited-state oxoiron(IV) species. This study provides insights into strategies to utilize light for efficient C-H bond activation by oxoiron(IV) complexes via the transient S=2 state.

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Poster Presentation : **PHYS.P-129**

Physical Chemistry

Event Hall THU 11:00~13:00

Study of Tyrosine Radical Formation and Dityrosine Cross-linking by Cu Ion and H_2O_2 Using Density Functional Theory.

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Alzheimer's disease (AD) is characterized by the deposition of self-assembled Amyloid-beta fibrils composed of highly stable and insoluble amyloid plaques in the neuropil. Al-Hilaly et al.[1] investigated the formation of dityrosine cross-links in the amyloid beta 42 peptide by covalent coupling of two tyrosine residues, which has been implied to play a key role in the development of the Alzheimer's disease. These dityrosines can be generated by reactive oxygen species catalyzed by Cu^{2+} ions.Using density functional theory, we studied this tyrosine radical formation with Cu ions and H_2O_2 to understand the tyrosine cross-linking mechanism. The calculations show that we can generate that tyrosine radical using Cu ions and H_2O_2 in a reaction mechanism involving Cu(III)OH. the TS energy of the reaction was 23.6 kcal/mol at the B3LYP/Def2-TZVPP level. This reaction energy shows that the above reaction can occur, and occurs slowly in water solvent condition.[1] Al-Hilaly et al. A central role for dityrosine crosslinking of Amyloid-β in Alzheimer's disease, Acta Neuropath. Commun. 2013, 1, 83.

Poster Presentation : **PHYS.P-130**

Physical Chemistry

Event Hall THU 11:00~13:00

Composite Silver Nanosurfaces with Dipole and Quadrupole Surface Plasmons Optimal for Emission Enhancements of Chromophores

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Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Metal-enhanced fluorescence (MEF) has been regarded promising in developing fluorescence-based analytical methods such as single molecule imaging, chemical sensing, etc. due to strong fluorescence enhancement and reduced photobleaching. MEF originates from the locally enlarged electric field around metal nanoparticles and plasmon-coupled emission by the excitation of surface plasmon resonance (SPR) of metal nanoparticles. The spectral overlap between the chromophore's emission and the SPR of metal nanoparticles is considered critical factor for the fluorescence enhancements. Dipole or quadrupole SPR modes of metal nanoparticles have been shown effective for fluorescence enhancements. However, the detailed investigation on the fluorescence enhancements and enhancement mechanisms between the dipole and quadrupole SPR modes of metal nanoparticles has not been reported yet. In this work, the fluorescence enhancements of several chromophores with the composite silver colloidal films (SCFs) prepared by homogeneous silver nanoparticles of specific small and large diameters were explored. The fluorescence signals of the chromophores were most largely enhanced with the composite SCFs with the specific ratios between the nanoparticles of dipole and quadrupole SPRs, where the combined (dipole and quadrupole) SPR bands of the SCFs are in good spectral overlap with the emission spectra of chromophores. For example, Alexa Fluor showed strong fluorescence enhancements with the composite SCFs than other chromophores, which indicates the great potential for the application in bioimaging and sensing. The fluorescence kinetics of the chromophores with the SCFs were also investigated by time-resolved fluorescence spectroscopy to show the mechanistic difference of MEF between the dipole and quadrupole SPRs of the composite SCFs.

Poster Presentation : **PHYS.P-131**

Physical Chemistry

Event Hall THU 11:00~13:00

Building a Miniature Digital Rectilinear Ion Trap Mass Spectrometer

Md Musleh Uddin Munshi, Han Bin Oh[1,*]

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[1]*Department of Chemistry, Sogang University, Korea*

We aim to build a miniaturized digital rectilinear ion trap (DRIT) mass spectrometer (~10x10x40 mm3) (Fig 1). Incorporation of digital technology in ion trap (Paul type, linear quadrupole) MS is not new. Recently, this got the most attention due to the advancement of digitization. We have already designed and manufactured the RIT based on the existing design of Ouyang et al. These RITs have geometries that are much simpler than hyperbolic Paul traps which enable tremendous control to manufacture. In addition, RITs show much higher trapping capabilities. Crucial advantage of the RIT based mass analyzers is the use of digital rectangular waveforms on the electrodes instead of classical rf-Sine waveforms. Besides, the mass scan is achieved by scanning the frequency while the voltage is held constant but not the opposite. Manipulation of the duty cycle of the trapping waveform and the excitation waveform allow us to carry out mass (m/z) isolation and CID MS respectively without the need of additional circuitry. Not to mention, RITs require much lower voltage (~600 Vp-p) to operate than Paul traps which helps to avoid electrical discharge. In this research, we employ commercially available software SIMION/SIMAX for simulation of ion motions inside RIT. This theoretical study is important to optimize crucial parameters further to build the instrument.

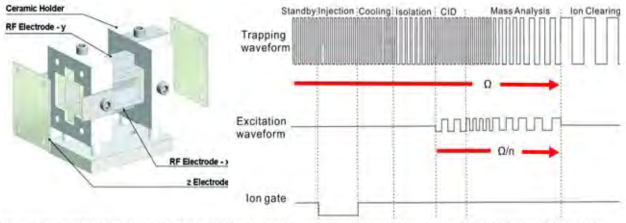

Fig 1 RIT assembly and the schematic of the experimental timing sequence adopted from Ouyang et al, Anal. Chem. 2004, 76, 16, 4595-4605 and Xu et al, J. Am. Soc. Mass Spectrom. 2014, 25, 556-562 respectively.

Poster Presentation : **PHYS.P-132**

Physical Chemistry

Event Hall THU 11:00~13:00

The Role of Axial Ligand of Cpd-I on the C-H Bond Activation: A DFT Study

Soobin Kwon, Yongho Kim*

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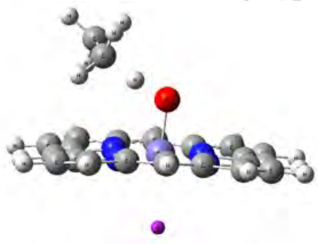
Cytochrome P450 enzymes are remarkably various oxygenation catalysts that are found throughout nature. The axial ligand of Cpd-I affects catalytic efficiency and plays an important role in hydroxylation. To elucidate the axial ligand effect, the C-H activation reaction by Cpd-I(X) (X= SCH3, H2O, Cl, Imidazole, etc.) was calculated with DFT. This study describes how the axial ligand of Cpd-I lowers the activation energy of the hydrogen atom transfer (HAT) reaction. In order to understand HAT mechanism, donor-acceptor interactions between axial ligand and Cpd-I, and between substrate and Cpd-I were calculated using the natural bond orbital analysis. We calculated spin-dependent linear free energy relation to test whether it can be used to elucidate the mechanism of the C-H bond activation.



Poster Presentation : **PHYS.P-133**

Physical Chemistry

Event Hall THU 11:00~13:00

Role of Electrochemical Reactions in the Degradation of Formamidinium Lead Halide Hybrid Perovskite Quantum Dots

YeJi Shin, Seog Joon Yoon*

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Organic-inorganic hybrid perovskites are widely utilized in solar driven chemistry such as photocatalysis, hydrogen evolution, and oxygen reduction. Hybrid perovskites contain various components with high polarity and/or charge values, which undergo transformations due to ion exchange, photoinduced phase segregation, or ion migration. These variable characteristics make perovskites “soft materials”. Meanwhile, optoelectronic devices often operate under electrochemical reactions in the presence of an electrical field. To examine the effect of this field on the material/photophysical properties of hybrid perovskites, hybrid $FAPbBr_3$ (FA^+: $CH(NH_2)_2^+$) perovskite quantum dots (PQDs) were synthesized. In this study, we report the spectroelectrochemical investigation of the hybrid $FAPbBr_3$ PQDs to understand the electrochemical stability and degradation process. We also found that the electrochemical condition played an important role in inducing defect-mediated oxidation/reduction reactions, changing the photophysical properties of hybrid PQDs, and causing their irreversible transformations to various lead halide plumbate complexes. These findings can help develop a strategy for enhancing the operational performance of PQDs for the solar driven chemistry.

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Poster Presentation : **PHYS.P-134**

Physical Chemistry

Event Hall THU 11:00~13:00

Twisted Intramolecular Charge Transfer of Stilbazolium Derivatives by Time-Resolved Raman Spectroscopy

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The intramolecular charge transfer (ICT) is one of fundamental chemical reactions where the charge transfers between the electron donor and acceptor groups often accompany structural changes of chromophores such as the rotation of the electron donor or acceptor group. The instantaneous structural changes of chromophore upon the ICT in the excited state have been studied by many time-resolved spectroscopic methods, where the twist of specific functional groups shows strong steric hindrance. For example, the ICT of (dimethylamino)stilbazolium derivatives with the functional group for the steric hindrance at the *ortho*- and *para*- positions from the twisting group were investigated by time-resolved fluorescence spectroscopy, where the dynamics with the *ortho*-isomer appears slower than the *para*-isomer. In this work, the detailed structural changes and ICT dynamics of stilbazolium derivatives were investigated by time-resolved electronic and vibrational spectroscopy. Two 4-N,N-diethylamino-N'-methyl stilbazolium tosylate (DEST) derivatives which consist of styrylpyridinium backbone and methyl group at the *ortho*- and *para*- position from the central ethylene group were synthesized. Twisted ICT of DEST isomers from FSRS measurements were probed by the changes in the skeletal vibrational modes of styrylpyridinium backbone in the 1500-1650 cm^{-1} range, and supported by the time-dependent density functional theory (TDDFT) simulations. The ICT dynamics of two DEST isomers were then interpreted as the rotational dynamics of diethylaminophenyl group (electron donor).

Poster Presentation : **PHYS.P-135**

Physical Chemistry

Event Hall THU 11:00~13:00

Improving V-Dock: Fast Generation and virtual screening of Novel Drug-like Molecules Using Machine-Learning-Based Docking Score and Molecular Optimization

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We propose a computational workflow to design novel drug-like molecules by combining the global optimization of molecular properties and protein-ligand docking with machine learning. However, most existing methods depend heavily on experimental data, and many targets do not have sufficient data to train reliable activity prediction models. To overcome this limitation, protein-ligand docking calculations must be performed using the limited data available. Such docking calculations during molecular generation require considerable computational time, preventing extensive exploration of the chemical space. To address this problem, we trained a machine-learning-based model that predicted the docking energy using SMILES to accelerate the molecular generation process. The docking program for training used Autodock GPU, Glide, and FRED. The performance of this model was verified with six proteins in the LIT-PCBA dataset. As a result, it was shown that this docking score prediction model not only reduces resources for docking, but also enables virtual screening. Docking scores could be accurately predicted using only a SMILES string. We combined this docking score prediction model with the global molecular property optimization approach, MolFinder, to find novel molecules exhibiting the desired properties with high values of predicted docking scores. We named this design approach V-dock. Using V-dock, we efficiently generated many novel molecules with high docking scores for a target protein, a similarity to the reference molecule, and desirable drug-like and bespoke properties, such as QED. The predicted docking scores of the generated molecules were verified by correlating them with the actual docking scores.

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Poster Presentation : **PHYS.P-136**
Physical Chemistry
Event Hall THU 11:00~13:00

Abnormality of catalysts in operational conditions with a high-level theory

Se-Jun Kim, Stefan Ringe[1], Hyungjun Kim[*]

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As the holy grail, the low-dimensional materials are on the stage for different catalytic reactions. In their operational conditions, it is well known that the dielectric properties of solvents modulate the electronic and optical behavior of catalysts. Although tremendous research to understand the dielectric effects on the low-dimensional materials has been carried out, the rarity of appropriate theories to resolve the complexity at a solid-liquid interface put obstacles in front of researchers. To overcome these limitations and unlock the origin of unexpected phenomena at this interface, we developed a new theoretical framework on the foundation of GW approximation and Bethe-Salpeter equation (BSE) with generalized Poisson equation. With the help of this methodology, we reproduced the intrinsic properties of catalysts well and found first time the signature that the interaction of the low-dimensional materials with the solvents leads to the anomaly of catalysts. Especially, the field effect by the polarization of solvents can be controlled universally by the dielectric environments. In addition, the quasiparticles are strongly correlated with the dielectric constants of solvents and the power law between the electrode and the electrolyte can be broken out in real environments. These results suggest concertedly that this theoretical model can provide mechanistic guidance toward unexplored chemical space.

Poster Presentation : **PHYS.P-137**

Physical Chemistry

Event Hall THU 11:00~13:00

Excited State Proton Transfer of Photoacids in Heterogeneous Environments studied by Time-Resolved Electronic and Vibrational Spectroscopy

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Reaction dynamics occurring in heterogeneous environments such as near the cell membranes or inside the protein complexes are of great importance in understanding many chemical and biological reactions. For example, chemical reactions inside the nanoscopic solvent pools of the reverse micelles are regarded as good model systems for studying heterogeneous reaction dynamics. Furthermore, the deep eutectic solvent mixtures are regarded as the emerging class of ionic liquids where the cationic and anionic solvent molecules are aligned with strong hydrogen bonding networks and show significant changes in many solvent polarities, including the melting point, viscosity, conductivity, etc.Excited-state dynamics of pyranine (HPTS) in the reverse micelles have been studied by time-resolved electronic spectroscopy, where the proton transfer and recombination dynamics appear strongly dependent on the size of micelles. The pyranine derivatives with weaker or stronger acidity, APTS (-NH2), and HPTA (-N(CH3)2) were also investigated in the heterogeneous environments of the reverse micelles. The deprotonation dynamics in the deep eutectic solvents, ethaline (2:1 mixture of ethylene glycol and choline chloride), and reline (2:1 mixture of ethylene glycol and urea) will also be studied by time-resolved electronic and vibrational spectroscopy to study reaction dynamics depending on the heterogeneous environments.

Poster Presentation : **PHYS.P-138**

Physical Chemistry

Event Hall THU 11:00~13:00

Calculations and simulations of UV-Vis absorption spectra in manganese- and iron-oxo complexes and their derivatives

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High-valent metal-oxo complexes are generally considered as key intermediates in biological and chemical catalytic oxidation reactions, and numerous manganese- and iron-oxo complexes have been successfully synthesized and characterized spectroscopically or structurally. Nam and coworkers performed experiments where a multiple-oxidant mechanism was supported in non-heme synthetic metal-oxo species oxidizing a substrate.[1] In such a mechanism, several oxidants can perform substrate oxidations simultaneously, and it therefore becomes difficult to confirm which of the intermediates is responsible for the UV-Vis absorption spectrum. Therefore, in this study, density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations have been performed to simulate the UV-Vis absorption spectra of a number of manganese- and iron-oxo complexes and their derivatives, which is crucial to the differentiation of the intermediates. At the PBE0 level of theory, TDDFT calculations on the triplet states of the Mn(V)-oxo and Mn(V)-hydroxo porphyrin complexes, with chloride ion as the auxiliary ligand, showed distinct UV-Vis absorption spectra. The low-energy absorption bands of the two complexes have different absorption origins. In the Mn(V)-oxo complex, the low-energy absorption band computed at ca. 840 nm is contributed by the ligand-to-ligand charge transfer (LLCT) transition from the chloride to the porphyrin moiety, whereas the one in the Mn(V)-hydroxo complex, which is located at ca. 720 nm, is mainly attributed to the intraligand (IL) transition of the porphyrin moiety. In addition to the Mn(V) complexes, the simulated UV-Vis absorption spectra of the sextet states of the Fe(III)-oxo, hydroxo and hydroperoxo complexes bearing tetramethylcyclam (TMC) ligand also show significant difference. While the Fe(III)-oxo complex gives a weak absorption band of ligand-to-metal charge transfer (LMCT) and metal-centered (MC) characters at ca. 350 nm, the Fe(III)-hydroxo complex exhibits an intense band of LMCT character at ca. 320 nm, and the Fe(III)-hydroperoxo complex shows a more red-shifted intense band of IL and LMCT characters at ca. 650 nm. The computational results of the current study help to establish a consistent, reliable and valuable

database for the photophysical properties of the manganese- and iron-oxo complexes and their derivatives. This database can further be used to confirm the transient intermediates by qualitative and quantitative comparisons with the experimental UV-Vis absorption spectra.**Reference**1.Nam, W.; Choi, S. K.; Lim, M. H.; Rohde, J. U.; Kim, I.; Kim, J.; Kim, C.; Que, L., Angew. Chem. Int. Edit. 2003, 42 (1), 109-111.

Poster Presentation : **PHYS.P-139**

Physical Chemistry

Event Hall THU 11:00~13:00

Plasmonic Catalytic Activity of Au@TiO_2–Au Core–Satellite Nanoassemblies

Joohwan Park, **Sangwoon Yoon**[1,*]

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A collective oscillation of conduction electrons, referred to as plasmon, governs the properties of gold nanoparticles (AuNPs). Plasmonic catalysis is derived from its nonradiative decay. The excited plasmon creates highly energetic electrons called hot carriers whose energy deviates from the thermal Fermi-Dirac distribution while it decays via electron-surface scattering. Transfer of those hot carriers to nearby molecules drives chemical reactions. In this respect, hot carrier generation efficiency is the key to enhancing the plasmonic catalytic activity. Previous studies revealed that the nanogaps promote the generation of hot carriers by relaxing the linear momentum conservation requirements. In this study, we aim to develop highly efficient plasmonic catalysts by fully utilizing the nanogaps between AuNPs. We cover the core AuNPs with very thin TiO_2 nanoshells (Au@TiO_2) and decorate them with satellite AuNPs. The resulting core-satellite nanoassembly structures have multiple, narrow nanogaps (~2 nm) between the core and satellite nanoparticles, filled with semiconductor materials which lengthen the lifetime of hot carriers. We explore the dye degradation and water splitting efficiency by the newly developed core-satellite plasmonic catalysts.

Poster Presentation : **PHYS.P-140**

Physical Chemistry

Event Hall THU 11:00~13:00

Effect of Nanoparticle Size on Plasmon-Driven Reaction Efficiency

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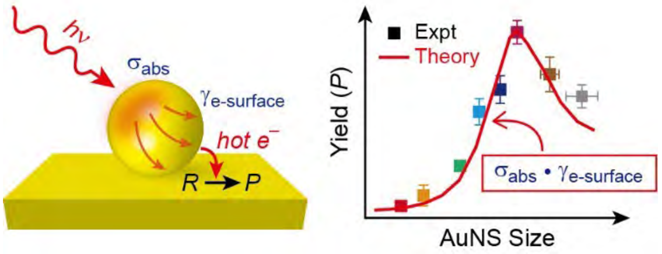
Chemistry, Chung-Ang University, Korea
[1]*Department of Chemistry, Chung-Ang University, Korea*

In recent few decades, interest in nanoparticles tremendously increased owing to having developed nanotechnology, and there are many applications using surface plasmon properties. Among them, hot electron generation plays a massive part in applications. Hot electron produced by non-radiative decay of surface plasmon transferred to the adsorbate and induced a reaction. Highly monodispersed CTAC capped AuNS, enabling investigation of the size dependence of surface plasmons. We investigate the effect of the nanoparticle size to on the reactivity of plasmon-driven reaction through decarboxylation of 4-mercaptobenzoic acid (MBA), which occurs in the nano-gap. The result shows a strange trend, increase reactivity with increasing size of nanoparticles, but the trend is reversed over 96 nm. There are two dominant factors that affects hot electron generation, absorption coefficient (σ_{Abs}) and hot electron generation efficiency derived from the Drude model. With the hypothesis that hot electron generation can be expressed as multiply σ_{Abs} and hot electron generation efficiency, this strange result is well-matched with hot electron generation.



Poster Presentation : **PHYS.P-141**

Physical Chemistry

Event Hall THU 11:00~13:00

An appraisal on the non-Condon effect based on the nonadiabatic effects: A time resolved spectroscopic study

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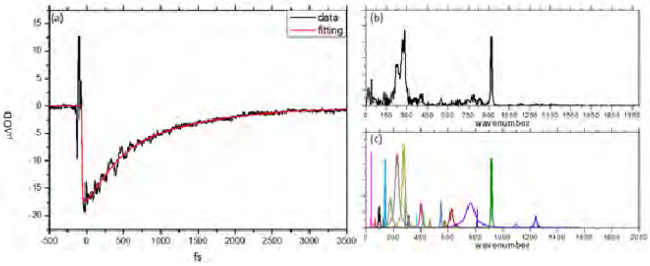
In the excited state chemical reaction, non-adiabatic transition occurs on two adiabatic surfaces placed close together. Conical intersections (CI) is known as an efficient method of non-adiabatic transition. Although it has an important role in understanding photochemistry, otherwise CI is rarely observed experimentally [1][2]. Here, we introduce 2,2′-dihydroxyazobenzene (2,2′- DHAB) as the CI occurs during the excited state intramolecular proton transfer in the condensed phase [3].Transient absorption (TA) signal (Figure1(a)) was acquired by the pump pulse around 400 nm and the probe at 750 nm with 18 fs time resolution, which give mostly the stimulated emission (SE) component. Vibrational spectrum was achieved by Fourier transform (Figure1(b)) and LPSVD (Figure1(c)) of residual of TA data. Vibrational peak at 920 cm< sup>-1< sup/> is solvent Raman of acetonitrile. Significant peak at 280 cm< sup>-1< sup/> is coherent wavepacket motion in the same phase in the entire wavelength range, which means non-Condon effect.A new hybrid exchange–correlation functional named CAM-B3LYP with 6-31+G** was employed for calculating the density functional theory (DFT) and time-dependent density functional theory (TD-DFT). All calculations were performed using the Gaussian 16 software. In the quantum calculation result, the oscillator strength of S< sub>0< sub/>→S< sub>1< sub/> enol transition is almost zero. But, the oscillator strength of S< sub>0< sub/>→S< sub>1< sub/> keto transition is 0.5741. REFERENCES[1] Jeong Sik Lim and Sang Kyu Kim, Nat. Chem. 2010; 2: 627-632.[2] Rose, T.S. and Zewail, A.H., J. Chem. Phys., 1998; 88: 6672-6673.[3] Yusuke Yoneda and Hiroshi Miyasaka, J. Phys. Chem. A, 2020; 124: 265-271.[4] Eom I, Joo T, Opt. Express 2014; 22: 30512-30519.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Poster Presentation : **PHYS.P-142**

Physical Chemistry

Event Hall THU 11:00~13:00

Non-stoichiometric Silver Telluride Colloidal Quantum Dots for Extended Short-Wavelength Infrared Emission and Photocurrent

Kwang Seob Jeong*, Haemin Song, Gahyeon Kim

Department of Chemistry, Korea University, Korea

Recently, nontoxic colloidal quantum dots(CQD) which show the optical property in the infrared region have been in demand due to their versatility in applications such as photodetectors and autonomous vehicles. Here, we present the non-stoichiometric AgxTe (x>2) CQDs that has the band-gap transition in the extended short wavelength infrared region, which is tunable by changing the ratio of Ag/Te. In addition, it was demonstrated that the air stability and structural rigidity can be improved by growing Ag2S as the shell. To prove the applicability, AgxTe CQDs was fabricated on the substrate, and the photocurrent and current density-voltage curve were measured. Under the infrared light at 78 K, the responsivity of the device exhibited 2.1 A/W at 0.63 V. The high detecting value with nontoxic components of AgxTe CQDs indicated that they have the potential to play the important role in various infrared optoelectronics such as bioimaging and telecommunications.

Poster Presentation : **PHYS.P-143**

Physical Chemistry

Event Hall THU 11:00~13:00

Colloidal Tellurium Nanowire Laser in the midwavelength infrared region

Gahyeon Kim, Kwang Seob Jeong[*]

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Bright colloidal infrared emitters have been attracted due to potentials for applications of the sensors, low-power light-emitting diodes (LEDs), and deep-tissue imaging. Here, we present the colloidal tellurium nanowires (Te NWs) which show the strong emission intensity in the midwavelength infrared region. As decreasing the temperature from room temperature to cryotemperature, the full-width-half-maximum (FWHM) becomes narrower and the emission intensity dramatically increases, which comes from lasing property. Furthermore, the intrinsic property of the Te NWs results in the second-harmonic generation (SHG) and third-harmonic generation (THG), which could expand the utility of infrared lasing. Surprisingly, the lasing is successfully measured with the antifreezing solvent at ~90 K and from the Te NWs embedded in a human cancer cell, indicating the potential for realizing deep-tissue imaging and thermotherapy.

Poster Presentation : **PHYS.P-144**

Physical Chemistry

Event Hall THU 11:00~13:00

Charge-Selective Ultraviolet Photodissociation Spectroscopy of Protonated Apo-Myoglobin Ions Stored in a Cryogenic Ion Trap

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The structural determination of large proteins by laser spectroscopy is one of the most challenging goals in physical chemistry. Here, We have obtained the charge-selective ultraviolet photodissociation (UVPD) spectra of protonated apo-myoglobin (aMb) ions produced by electrospray ionization and stored in a cryogenic ion trap. The UVPD spectra exhibited distinct spectral features, which vary depending on the charge state of aMb. This study demonstrates that cryogenic ion spectroscopy is a powerful tool to obtain charge-selective UV spectra of large protein ions in the gas phase.

Poster Presentation : **PHYS.P-145**

Physical Chemistry

Event Hall THU 11:00~13:00

Direct Formation of alcohols from Photocatalytic partial oxidation of methane over TiO_2 modified by FeO_x

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[2]*Department of Chemistry, Ajou University, Korea*

Methane has a symmetrical tetrahedral structure with four completely equal C-H bonds. Thermodynamically, the initiation of the reaction requires an energy-intensive reaction due to the strong C-H bond (434 kJ/mol), but such a harsh condition is detrimental for the reaction product. Photocatalytic partial oxidation could provide a chance to drive the reaction selectively with photons rather than non-selective high-temperature reaction conditions. Therefore, we report the selective oxidation of methane to methanol on TiO_2 Nanosheet and P25 supported iron species using H_2O_2 as the oxidant. For the light source, UV light of $5mW/cm^3$ was used for the photocatalytic process with pressures of 4 and 8 bar. The structure, composition, and optical properties of FeO_x/TiO_2 were characterized by XRD, SEM, UV–vis spectroscopy and XPS. Meanwhile, to investigate the presence of the methanol, FID, Mass spectrometry and NMR analysis was used. We showed that increasing the loading of FeO_x on TiO_2 influenced the amount of alcohol produced. Besides, with higher concentrations of H_2O_2, the amount of O_2 evolved increased comparatively which enhance the alcohol production to a certain extent. Especially, there were great disparities between the amount of product for P25 and Nanosheet with FeO_x/TiO_2(P25) providing a higher amount of products. This difference could have been the result of the disparities in surface structures between P25 and TiO_2 nanosheet which could influence the selectivity of the products. The exact nature of the reaction pathway and influence of various conditions is under further investigation.

Poster Presentation : **PHYS.P-146**

Physical Chemistry

Event Hall THU 11:00~13:00

Development of process for hydrogen production without CO_2 emission through direct catalytic pyrolysis of CH_4 using liquid metal catalyst

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[2]*Department of Chemistry, Ajou University, Korea*

Direct catalytic methane pyrolysis is attracting method for hydrogen production with increasing demand for reducing the CO_2 emission. Although steam methane reforming (SMR) effectively produces hydrogen than any other routes, emitted CO_2 by this process makes additional cost for capturing and sequestration(CCS). In this point of view, methane direct decomposition can be a good alternative for hydrogen production, which products from reaction being hydrogen and solid carbon. Also, since carbon floats on the liquid catalyst, it is beneficial to use liquid catalyst for separating the catalyst and the solid carbon. It can prevent a deactivation of the catalyst when carbon grows on the surface of solid catalyst during the reaction. In this report, we mixed active metal (Ni) with high melting point and a low melting point metal (Sn) as the solvent for methane decomposition. We achieved a 20% conversion rate with 14 ml Ni-Sn-based liquid metal for a small scale of bubble column reactor. By adjusting various variables such as, residence time, bubble size, structure of reactor, and the content of active metal, we estabilished factors affecting the methane conversion. In particular, the liquid metal catalyst was controlled by the size of the bubble and the residence time. With this factor, we eventually achieved a methane conversion rate increased above 90% with 14 ml Ni-Sn-based liquid metal.

Poster Presentation : **PHYS.P-147**

Physical Chemistry

Event Hall THU 11:00~13:00

Photoelectrochemical CO_2 Reduction Using an Efficient Bismuth doped-TiO_2 Photoanode and Pt-dark cathode

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CO_2 is generated by artificial methods such as combustion of fossil fuels. Therefore, there is a need for a sustainable and eco-friendly CO_2 treatment. In terms of utilization, if CO_2 can be converted into another material using sunlight, it can be used in a good way. Various n-type semiconductor nanostructures have been utilized as a photoelectrode for PEC CO_2 reduction. Especially, TiO_2 is abundant, nontoxic, cost-effective, stable and has proper bandgap energy (3.2 eV) which is suitable for CO_2 reduction under sun light. For TiO_2 photoanodes studied for PEC CO_2 reduction, there are several problems. First, to solve this problem, 1D TiO_2 is beneficial for efficient separation of photogenerated charge carriers along different directions on the rod/wire/tube. Second, using appropriate co-catalysts has been demonstrated to be an effective strategy in suppressing the surface electron–hole pair recombination and enhancing the PEC performances of photoanodes. Bismuth is a candidate as a co-catalyst in energy storage and conversion systems. It can effectively improve the activity of photocatalysts by the surface plasmon resonance effect, help separate electron–hole pairs, and extend the carrier life, as has been reported in previous studies.All of data demonstrate that doping Bismuth single atom enhance photoelectrochemical efficiency. In chronoamperometry, Bi-TiO_2 nanorods showed four times higher photocurrent density than TiO_2 nanorods. And it was maintained for a long time (4h) to show the stability of the photoanode. Bi-TNR had a slight decrease in band gap compared to TNR. And it is helpful using solar light because of the ratio of solar light.

Poster Presentation : **PHYS.P-148**

Physical Chemistry

Event Hall THU 11:00~13:00

Self-Doped HgSe Colloidal Quantum Dots as a Promising Material of Multifunctional Sensor

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The self-doped HgSe nanocrystals with a doubly occupied quantum state (DOQS) are extremely sensitive to the surface charge because the electrons in DOQS are spatially delocalized at the surface of the nanocrystal. Here, we present the thin-film transistors(TFT) fabricated with the self-doped quantum dots that can be used as a sensor for the three types of targets; environmental gases (CO_2 gas, NO gas, and H_2S gas); mid-IR photon; and biothiol (L-cysteine) molecules. The TFT can detect the small photential change caused by the gas molecules. Furthermore, the threshold voltage shift in the transfer characteristic of CO_2 gas proves that the molecules are physisorbed on the surface of TFT. The target molecules are quantitatively evaluated, and the detection limits for CO_2 and L-cysteine are 250 ppm and 10 nM, respectively. The comparable performance of self-doped TFT with commercial detectors suggests the possibility of utilizing the DOQS nanocrystals as high-performance sensors.

Poster Presentation : **PHYS.P-149**

Physical Chemistry

Event Hall THU 11:00~13:00

MXene/Pt composites with superior hydrogen evolution performance in alkaline or acidic condition

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[1]*Department of Chemistry, Gyeongsang National University, Korea*

Materials with a 2D structure are expensive or complicated to make, so research to improve them is being actively conducted. Among of them, MXene, a titanium carbide/nitride 2D structural nanosheet, has excellent physical durability, electromagnetic wave shielding, energy storage capacity and thermal conductivity. Because of its effect of the internal multi-reflection from the multi-layered structure. We synthesized MXene/Pt composites using the pulsed laser irradiation (wavelength 532nm and power 90mJ). The laser synthesis method is an eco-friendly method that does not generate by-products and sufficiently improve the limitations of the two-dimensional structure. From a variety of analytical techniques such as SEM, TEM, XRD, XPS and ICP and soon, we observed the well-made MXene/Pt composites. Furthermore, we tried to measure the electro-conversion efficiency as catalysts with controlling the laser irradiation time.

Poster Presentation : **PHYS.P-150**

Physical Chemistry

Event Hall THU 11:00~13:00

Interface engineering of Ni-Fe layered double hydroxide via pulsed laser ablation for efficient electrochemical water splitting

Sieon Jung, Myong Yong Choi[1,*], Seung Jun Lee[1,*], Yiseul Yu[*], Shreyanka Shankar Naik[2,*]

Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*
[2]*Chemistry, Gyeongsang National University, Korea*

As an ideal technology for the H_2 fuel production, electrochemical overall water splitting (OWS) is considered as a clean and promising technique to generate H_2 form the inexhaustibility sources. OWS consists of two half-electrochemical reactions, the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). In this work, we study an interface engineering strategy to fabricate an effective bifunctional Ni-Fe layered double hydroxides (LDHs) electrocatalyst via pulsed laser ablation in water as solvent for water-splitting process. The intrinsic physical and chemical characteristics of the synthesized Ni-Fe LDHs were characterized by various analytical techniques such as FT-IR, XRD, FE-SEM, EDS mapping, and XPS. The optimal proportion of Ni-Fe LDH exhibit a lowest OER overpotential of 306 mV at 10 mA cm^{-2} in 1.0 M KOH with excellent durability over 5 h. This study reveals the optimization of the structure and component LDH proportion ratios in Ni-Fe which could modulate the electronic structure as an energy-efficient multifunctional electrocatalysts for OWS.

Poster Presentation : **PHYS.P-151**

Physical Chemistry

Event Hall THU 11:00~13:00

Nanogap-tailored strategy of gold nanoparticles by pulsed laser process for SERS applications

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[1]*Department of Chemistry, Gyeongsang National University, Korea*
[2]*Department of Education Chemistry, Gyeongsang National University, Korea*

Herein, gold nanoparticles (Au NPs) were synthesized by pulsed laser ablation (PLAL) in a mixed-phase solvent of acetonitrile and water. The size of Au NPs and the number of graphitic carbon (GC) layers were controlled by varying the ratio of the solvent mixture. The surface-enhanced Raman scattering (SERS) of the Au NPs was investigated using 10−3 M 4-aminobenzenethiol (4-ABT) and 10−4 M 4-nitrobenzenethiol (4-NBT) as probe molecules. The SERS activity strongly depended on the nanogaps between particles owing to the formation of hot spots. In the present work, the nanogaps were controlled by changing the amount of GC layers. No GC layers were produced in water, resulting low SERS intensity. In contrast, Au NPs prepared in 30 vol% of acetonitrile showed significant SERS enhancement, which was attributed to the optimal size of the GC-coated NPs and a reasonable gap between them. The obtained results revealed that Au NPs produced by PLAL could be applied in SERS-based microsensors.

Poster Presentation : **PHYS.P-152**

Physical Chemistry

Event Hall THU 11:00~13:00

Rapid Production of CuPd Alloys via Pulsed Laser Process for Hydrazine-Assisted Energy-Saving Hydrogen Fuel Generation

Yu Jeong Jeong, Shreyanka Shankar Naik, Yiseul Yu, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Electrocatalytic water splitting for H_2 generation is one of the sustainable and proficient approaches but still limited by the kinetically sluggish oxygen evolution reaction (OER). An effective approach to significantly decrease the electricity utilization of water electrolysis is to substitute the OER with anodic hydrazine oxidation reaction (HzOR) due to the lower standard oxidation potential of −0.33 V. The semiconductor and absorption characteristics of Cu, interlacing by Pd^{2+} solution on the Pd surface by pulsed laser ablation (PLA) in methanol, are modified selectively to optimize cathodic hydrogen evolution reaction (HER) and anodic HzOR performance through alloying. The optimal proportion of Cu1Pd3/C exhibits exceptional HER activity with a low overpotential of 0.315 V at 10 mA/cm^2 in 1.0 M KOH electrolyte, concurrently delivering an ultralow overpotential of 0.56 V for HzOR in 0.5 M N_2H_4/1.0 M KOH. The present report advances the competent CuPd alloys as a multifunctional electrocatalysts via HzOR-assisted energy-efficient electrolyzer for H_2 fuel production.

Poster Presentation : **PHYS.P-153**

Physical Chemistry

Event Hall THU 11:00~13:00

Anomalous Active Motion of Cargo-Motor Multiplex in Sick Neurons

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Department of Chemistry, Chung-Ang University, Korea
[1]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

Microtubules, major components of the eukaryotic cytoskeleton, serve as intracellular roads on which motor proteins transport cargos such as neurotransmitters, proteins, nucleic acids, and even nanoparticles. Their stability is modulated by the phosphorylation state of tau proteins invaded in the microtubule. In sick or old neurons, the tau proteins are highly phosphorylated, detach from the microtubule, and then aggregate to form intracellular neurofibrillary tangles, the primary marker of Alzheimer's disease. However, we still do not know how the stability of the microtubule, or tau protein aggregation, affects in vivo motion of cargo carried by motor proteins along the microtubule. Here, we report that ballistic transport of the cargo-motor protein complex is strongly suppressed by tau protein aggregation caused by hyper-phosphorylation. We accurately track and analyze microtubule-based motion of individual vesicle-motor protein multiplexes in forskolin-treated, sick neurons. Under hyper-phosphorylation, the vesicle-motor multiplex exhibits seemingly passive random motion showing strong heterogeneity in the diffusion coefficient with both static and dynamic components. We provide a simultaneous, quantitative explanation of the experimental results for the mean squared displacement, the non-Gaussian parameter, and the displacement distribution of the in vivo vesicle motion in sick neurons, comparing the results with the results of vesicle motion in healthy neuronal cells. Our comparative analyses clearly show that, on the microtubules destabilized by phosphorylation of tau proteins, vesicle-motor protein complex's motion slows down due to the strong suppression of unidirectional, ballistic motion, or the fast long-distance vesicle transport, which suggests a new mechanism of neurodegenerative diseases.

Poster Presentation : **PHYS.P-154**

Physical Chemistry

Event Hall THU 11:00~13:00

Non-classical enzymatic kinetics of alkaline phosphatase

Sanggeun Song, Ji-Hyun Kim*, Jaeyoung Sung*

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We investigated the non-classical enzyme kinetics of alkaline phosphatase under enzyme-rich condition. From this study, we found that high enzyme concentration, which cannot be treated by conventional Michaelis-Menten kinetics, can provide valuable information about dynamics and mechanism of enzyme reaction. With help of the experiment using conventional spectroscopic techniques, we discovered that alkaline phosphatase does not follow the classical Michaelis-Menten kinetics; the enzyme-substrate complex lifetime distribution shows super-Poisson character. To demonstrate the dynamics of enzymatic process, pseudo-first order renewal enzyme kinetics model was used. From this model, we could extract the enzyme-substrate complex lifetime distribution from time-dependent profile of product concentration under high concentration of enzyme. Based on this enzyme-substrate complex lifetime distribution, we numerically solved the non-classical kinetic equations and compared with experimental data under various concentration of enzyme and substrate. Furthermore, we developed the stochastic simulation algorithm for non-classical enzyme reaction process with arbitrary concentration of enzyme and substrate, which provides the stochastic evolution of enzyme process. From this approach, one can easily identify the non-classical kinetics or turnover mechanism of enzyme process without using single molecule spectroscopy.

Poster Presentation : **PHYS.P-155**

Physical Chemistry

Event Hall THU 11:00~13:00

Heterogeneous transport dynamics of synaptic vesicles at presynaptic terminals

Gyunam Park, Ji-Hyun Kim*, Jaeyoung Sung*

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Synaptic vesicle motion within presynaptic terminals is an essential process underlying neuronal communication. However, complex vesicle motion and its effects on synaptic transmission are poorly understood. Here, we investigate the motion of individual synaptic vesicles by using three-dimensional tracking. We find the fusion time of synaptic vesicles does not simply increase with their initial distance from the fusion site, despite similar instantaneous speed for all vesicles. And synaptic vesicles show common behavior of bounded motion when arriving at fusion domain. We classify synaptic vesicles into two type. Type 1 is synaptic vesicles that arrived at the fusion domain before the neuronal stimulation (one-step firing), on the other hand, Type 2 is synaptic vesicles that arrived at the fusion domain after the neuronal stimulation (two-step firing). We investigate distributions of time taken for each step, magnitude of net displacement and correlation between the two. We extract information about transport dynamics of type 2 synaptic vesicles using first passage time analysis. We find that mean drift speed of synaptic vesicles increases upon the neuronal stimulation.

Poster Presentation : **PHYS.P-156**

Physical Chemistry

Event Hall THU 11:00~13:00

Statistical mechanics approach to DNA nanostar phase separation

In-Chun Jeong, Ji-Hyun Kim, Jaeyoung Sung*

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Phase separation causing the formation of membraneless droplets in living cells has been known as playing a crucial role in various biological processes including transcriptional regulation, signal transduction, and even pathogenic aggregation related to neurodegenerative diseases. To reveal underlying mechanism of how membraneless compartments are formed by phase separation, a lot of experimental studies have been conducted in various systems. DNA nanostars, consisting of multiple DNA strands, each of which has two sticky ends, have been widely used to investigate the phase separation phenomena because molecular properties of DNA nanostars such as valency or flexibility can be easily modulated. Although there have been various studies to observe the phase separation of DNA nanostars, its quantitative understanding has yet to be achieved. Here, we propose a new approach based on the partition functions of DNA nanostars at diluted phase and condensed phase. This approach enables a quantitative explanation of the DNA nanostar phase diagrams modulated by various factors such as number of association sites, temperature, flexibility, and salt concentration, and the extraction of the sticky end-mediated association free energy of DNA nanostars at condensed phase, which clearly shows why the widely used Wertheim theory fails at the condensed phase of DNA nanostars.

Poster Presentation : **PHYS.P-157**

Physical Chemistry

Event Hall THU 11:00~13:00

Stochastic Kinetics of Nanocatalytic Systems

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Catalytic reaction events occurring on the surface of a nanoparticle constitute a complex stochastic process. Although advances in modern single-molecule experiments enable direct measurements of individual catalytic turnover events occurring on a segment of a single nanoparticle, we do not yet know how to measure the number of catalytic sites in each segment or how the catalytic turnover counting statistics and the catalytic turnover time distribution are related to the microscopic dynamics of catalytic reactions. Here, we address these issues by presenting a stochastic kinetics for nanoparticle catalytic systems. We propose a new experimental measure of the number of catalytic sites in terms of the mean and variance of the catalytic event count. By considering three types of nanocatalytic systems, we investigate how the mean, the variance, and the distribution of the catalytic turnover time depend on the catalytic reaction dynamics, the heterogeneity of catalytic activity, and communication among catalytic sites. This work enables accurate quantitative analyses of single-molecule experiments for nanocatalytic systems and enzymes with multiple catalytic sites.

Poster Presentation : **PHYS.P-158**

Physical Chemistry

Event Hall THU 11:00~13:00

Topology analysis of non-renewal system using turnover time correlation

Heemo Yang, Ji-Hyun Kim*, Jaeyoung Sung*

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Advances in single molecule techniques enable to access information about the heterogeneity in single enzyme activity beyond the ensemble measurement. Based on the improvement of space and time resolution, attempts have been made to identify a fluctuation of the system network using a non-renewal process with hidden variable for counting statistics that cannot be explained by renewal process. However, due to the theoretical absence of the first-passage time distribution of the non-renewal process, studies on how the fluctuation of turnover time correction and first-passage time, which exist in experiments but cannot be explained under the assumption of a renewal process, are insufficient. This research is about the methodology and the difference when the system is generalized into a non-renewal process beyond the conditions of the renewal process. This difference is expected to be used as an important tool for experimental analysis, providing the most important parameters to consider outside the moments of the steady-state turnover time distribution to model and understand networks of complex systems generally described only by non-renewal processes.

Poster Presentation : **PHYS.P-159**

Physical Chemistry

Event Hall THU 11:00~13:00

AuPtCu nanoalloy electrocatalysts produced via pulsed laser techniques with boosted Reaction kinetics for formic acid oxidation

Yeryeong Lee, Yiseul Yu, Seung Jun Lee[1], Theerthagiri Jayaraman[1], Myong Yong Choi[1,*]

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In the method of water electrolysis, the process of storing highly explosive hydrogen gas is not simple. On the other hand, formic acid aqueous solution has no possibility of combustion or explosion, so it has excellent stability and being studied a lot in the field of fuel cells. In formic acid oxidation, formic acid solution is decomposed into carbon dioxide, generating hydrogen ions and electrons. It mainly occurs through the mechanism of two pathways, either decomposed without forming CO or decomposed to form an intermediate CO. In this study, we prepared a catalyst suitable for a formic acid fuel cell using an eco-friendly pulsed laser without using a reducing agent or surfactant. Electrocatalytic activity was studied by making alloys by ratio using Au, Pt, and Cu, which are often used in formic acid oxidation research. The produced material was analyzed using UV-vis, X-ray diffractometer (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Further, electrochemical properties were analyzed through cyclic voltammetry (CV) and chromoamperometry (CA). Did Through the formic acid oxidation reaction, it was found that AuPtCu was suitable as a catalyst for formic acid fuel cells. The present study validates the feasibility of AuPtCu alloys for stimulating direct formic acid fuel cells in the future to achieve an expected as power sources of portable devices.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-160**

Physical Chemistry

Event Hall THU 11:00~13:00

Analysis of micelle growth dynamics

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[1]*Department of Chemistry, Kangwon National University, Korea*

Sodium Laurylethoxysulfate (SLES) is a fundamental ingredient in a wide range of surfactant products and the mapping of its aggregation dynamics can help to understand many biological and industrial processes. With molecular dynamics(MD) simulation, we observed SLES micelle formation processes in water under different SLES concentrations (3, 5 ,7%). Further, we developed a mathematical model and statistical theories of growing micelles, providing a quantitative understanding of size dependent growth rate and dynamic equilibrium, constantly reforming and dissolving.

Poster Presentation : **PHYS.P-161**

Physical Chemistry

Event Hall THU 11:00~13:00

Evaluation of multiple docking programs for various sets of protein-ligand complexes

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The most popular molecular docking in modern structure-based drug design can predict interactions between proteins and ligands and significantly shorten drug design time. In this study, various sets of protein ligand validation tests present at the bindingdb site were calculated using five docking programs (autodock, autodock-vina, glide, fred, ucsfdock6).Through this, the optimal binding posture and binding affinity between the protein and the ligand could be obtained. By comparing the above result values and actual values, the optimal protein-ligand docking program can be found. This work is expected to provide useful information for successfully applying these docking tools to various requirements and targets

Poster Presentation : **PHYS.P-162**

Physical Chemistry

Event Hall THU 11:00~13:00

The chemical fluctuation theorem governing expression, protein maturation and annihilation

Jin Hyung Kim, **Ji-Hyun Kim***, **Jaeyoung Sung***

Department of Chemistry, Chung-Ang University, Korea

Fluorescence protein is a powerful probe of gene expression dynamics in living cells. It is known that these protein emit fluorescence after slow maturation processes; however, it is not known how this maturation process affects the protein level which can be probed by fluorescent proteins. Here, we address this issue by presenting a new type of the chemical fluctuation theorem (CFT) that exactly holds for proteins with general gene expression and maturation dynamics. Using the CFT, we present the first, accurate relationship between the gene expression and maturation dynamics to experimental observables including the mean and variance of matured protein level in living cells. We also investigate how dynamic, cell-to-cell fluctuation of the gene expression dynamics and non-exponential lifetime distributions of protein affect these experimental observables. This work enables accurate, quantitative understanding of gene expression and protein maturation dynamics in living cells.

Poster Presentation : **PHYS.P-163**

Physical Chemistry

Event Hall THU 11:00~13:00

Facile synthesis of Co3C using pulsed laser ablation for electrochemical hydrogen fuel generation

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[1]*Gyeongsang National University, Korea*

Electrochemical water splitting provides a promising strategy for effective and sustainable hydrogen production, and one of the immediate challenges is the availability of low-cost and efficient electrocatalysts for the hydrogen evolution reaction (HER). There is a need to develop low-cost, stable, and efficient electrocatalysis. Transition metal carbide (TMC), which behaves like platinum, has attracted interest in the development of non-noble metal-based electrocatalysts. In this work, we used earth abundant cobalt and successfully produced cobalt carbide (Co_3C) through pulsed laser ablation in acetone as solvent as well as carbon source. The intrinsic physical and chemical characteristics of the synthesized Co_3C materials was characterized by various analytical techniques such as XRD, FE-SEM, EDS, and HRTEM. The electrocatalytic performance toward hydrogen production was examined via voltammetry techniques. This work provides facile and advanced strategy in the preparation and modulation of TMC electrocatalysts toward high-performance HER.

Poster Presentation : **PHYS.P-164**

Physical Chemistry

Event Hall THU 11:00~13:00

Comparative Study of Alkanethiol and N-heterocyclic Carbene Self-Assembled Monolayers on Au(111)

Young Ji Son, Sicheon Seong, Hyun Su Oh, Haeri Kim, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

For the three decades, research of self-assembled monolayers has been developed based on sulfur as the chemical anchor with a gold substrate for the applications of organic electronic devices such as organic light-emitting diodes (OLED) and organic field-effect transistors (OFETs), organic memory, and solar cells. However, using sulfur as a bonding atom with a gold substrate has raised low thermal and oxidative stability problems. N-heterocyclic carbene (NHC) with two heteroatoms of nitrogen increasing stability has been proposed as an excellent alternative to forming SAMs because NHC-based SAMs on Au(111) has higher thermal/chemical stability than standard thiol-based SAMs. In this study, we synthesized dimethyloxy benzoimidazolium hydrocarbonate (C8-Me-NHC-HCO3) molecules containing octyloxy alkyl chain and methyl wing tips to form SAMs on Au(111). Furthermore, we observed the structural and electrochemical differences between NHCs and 1-decanethiol (DT) SAMs compared with alkanethiol, which has a similar molecular length to C8-Me-NHC-HCO3 molecules using scanning tunneling microscopy (STM) and cyclic voltammetry (CV). Unlike decanethiol SAMs in which molecules formed c(4x2) unit cells, C8-Me-NHC-HCO3 SAMs exhibit three local orientation arrangements whose unit cells defined (√19x6) structure, and the size and molecular spacing of the molecules are much larger and broader than DT SAMs. In the CV measurement, the reductive desorption peak of C8-Me-NHC-HCO3 SAMs was detected at -991 mV (10 min) and -930 (1 h and 24 h). In the case of DT SAMs (1 h), RD peak was observed at -1100 mV. In the case of C8-Me-NHC-HCO3 SAMs formed under 10 min conditions, NHC molecules form a densely packed structure that is more difficult to detach than other long-time deposition conditions. In addition, DT SAMs have a highly ordered surface structure due to sufficient van der Waals, resulting in molecular desorption in a sufficiently negative potential.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-165**

Physical Chemistry

Event Hall THU 11:00~13:00

Surface Structure and Interfacial Electrical Properties of Alicyclic Thiolate and Selenolate Self-Assembled Monolayers on Au(111)

Sicheon Seong, Young Ji Son, Haeri Kim, Hyun Su Oh, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are ultrathin films formed by spontaneous adsorption and 2-dimensional self-assembly of organic molecules on metal or semiconductor substrates. They have largely been studied for past few decades because of their ability to modify physical and chemical properties of solid surface and interfaces. Although thiols have long been employed as the most common anchoring group, selenols have recently been studied as alternatives to thiols. At saturation coverage, alkanethiolate SAMs on Au(111) form closely packed hexagonal structure which can be represented as $(\sqrt{3} \times \sqrt{3})R30°$ or $c(4 \times 2)$ unit cell. On the other hand, alkaneselenolate SAMs formed markedly different structure from that of alkanethiols, exhibiting missing-row phases. Alicyclic SAMs have flexible aliphatic ring, and thus provide interesting self-assembly circumstances based on their axial and equatorial isomers. Well-ordered cyclohexanethiolate (CYH-S) SAMs showed zig-zag molecular rows with alternating molecular height. However, there have been no reports about selenolate SAMs with alicyclic backbone so far. To understand the effect of anchoring group on the formation and structure of alicyclic SAMs, CYH-S and cyclohexaneselenolate (CYH-Se) SAMs were prepared by solution and vapor phase deposition and discussed in detail with molecularly resolved scanning tunneling microscopy (STM) images. In addition, the electric interfacial properties of the SAMs were investigated by using Kelvin probe force microscopy (KPFM).

Poster Presentation : **PHYS.P-166**

Physical Chemistry

Event Hall THU 11:00~13:00

2D IR Study of the aggregation pathway of hIAPP oligomers

Hyejin Kwon, Jin Gyu Seol, Yung sam Kim*

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Type 2 diabetes (T2D) is a disease in which human islet amyloid polypeptide (hIAPP) amyloid deposits attack β-cells, causing insulin production problems and the loss of blood sugar control. Although the formation process of hIAPP deposits has been studied for several decades, the early stage of the aggregation mechanism is not fully understood due to the transient nature of intermediate oligomers. In this regard, we slowed down the aggregation process by lowering the sample temperature and observed the aggregation process in detail. The aggregation process was clearly observed by 2D IR to be reversible at the early stage aggregation.

Poster Presentation : **PHYS.P-167**

Physical Chemistry

Event Hall THU 11:00~13:00

Hydration level dependent diffusional heterogeneity of water molecules confined between lipid bilayer membranes

Minho Lee, Euihyun Lee[1], Ji-Hyun Kim, Minhaeng Cho[2], Jaeyoung Sung[*]

Department of Chemistry, Chung-Ang University, Korea
[1]*Department of Chemistry and Biochemistry, University of Texas at Austin, United States*
[2]*Department of Chemistry, Korea University, Korea*

Transport dynamics of water near lipid bilayer membranes largely deviates from that of bulk water mainly because of the intermolecular interaction between water molecules and lipid head groups. Although it is well known that the mean square of lateral water displacements exhibits transiently anomalous diffusion followed by normal diffusive motion with diffusion coefficients smaller than in the bulk state, the non-Gaussian character of the transport dynamics, reflecting diffusional heterogeneity of lateral water motion, has yet to be quantitatively investigated. In this work, we study the non-Gaussian transport dynamics of water molecules confined between 1,2-dimyristoyl-sn-glycero-3-phosphorylcholine (DMPC) bilayer membranes using extensive molecular dynamics simulations1 at various hydration levels. The long-time tail of the non-Gaussian parameter for the lateral water displacement is contributed by the effective caging time and the term originating from the diffusion coefficient fluctuation.2 We find that the latter is the main contributor to the non-Gaussian parameter in the current lipid bilayer system and its magnitude increases with lipid to water number ratio. In particular, the non-Gaussian transport dynamics of water in the low hydration level system where lipid head groups in different membranes overlap each other exhibits distinctly different features from that in the relatively high hydration level system where lipid head groups in different membranes are well separated from each other. 1E. Lee, A. Kundu, J. Jeon and M. Cho, J. Chem. Phys., 2019, 151, 114705.2S. Song, S. J. Park, M. Kim, J. S. Kim, B. J. Sung, S. Lee, J. H. Kim and J. Sung, Proc. Natl. Acad. Sci. U. S. A., 2019, 116, 12733–12742.

Poster Presentation : **PHYS.P-168**

Physical Chemistry

Event Hall THU 11:00~13:00

Reconstruction of lossless molecular representations

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SMILES is the most dominant molecular representation used in AI-based chemical applications, but is also responsible for certain issues associated with its internal structure.Here, we exploit the idea that structural fingerprints may be used as efficient alternatives to unique molecular representations.For this purpose, we assessed the conversion efficiency of fingerprints back to the molecules.We successfully reconstructed molecules by achieving high level of accuracy.Our approach the, therefore,ngs structural fingerprints into play as strong representational tools in chemical NLP applications by restoring the connectivity information that is lost during the fingerprint transformation.This comprehensive study addresses the major limitation of structural fingerprints which precludes their implementations in NLP models. Our findings should enhance the efficiency of the models in generative and translational fields.

Poster Presentation : **PHYS.P-169**

Physical Chemistry

Event Hall THU 11:00~13:00

Correlation between cell-cell interaction and membrane fluidity

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Department of Chemistry, Chung-Ang University, Korea

Cells sense and respond to mechanical forces that are exerted by interaction with neighboring cells, regulating cell growth, adhesion and immune response. To understand the force-sensitive biological processes, it is indispensable to measure the cellular forces generated by ligand-receptor interaction between cells. However, it is almost impossible to quantify the ligand-receptor interaction in their native fluidic environment because of several technical limitations. Here, we measured the interaction between the ligands in the mobility-adjustable artificial cell membrane and the receptors of living cells by employing a double-stranded DNA-based force sensor. We found that the ligand-receptor interaction in the fluidic environment is significantly stronger than the one in the less mobile environment. This result would contribute to enhance the understanding of the ligand-receptor interaction controlled by the fluidity of their environment.

Poster Presentation : **PHYS.P-170**

Physical Chemistry

Event Hall THU 11:00~13:00

Phase engineering of nanostructured copper sulfide by pulsed laser ablation in liquids and its multifunctional photo-electrocatalytic activity

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Department of Chemistry, Gyeongsang National University, Korea

Highly efficient and less expensive electrocatalysts are of great importance to create a sustainable future energy source. Herein, facile pulsed laser ablation in the liquid synthesis route was utilized for the fabrication of phase-engineered Cu_xS_y nanospheres. The activity of these catalysts was assessed by examining the hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and methanol oxidation reaction (MOR). Consequently, low overpotentials of 390 mV (HER) for sulfur-rich and 440 mV (OER) for copper-rich samples were achieved in alkaline media. The selectivity of Cu over methanol and the high number of electrochemically accessible active sites equal to 7.9×10^{16} promoted the MOR with a current density of 28.3 mA/cm^2. Finally, enhanced OER catalytic activity was obtained under light irradiation due to the large light absorption coefficients of the synthesized electrocatalysts, which facilitated electron transfer at the electrode-electrolyte interface.

Poster Presentation : **PHYS.P-171**

Physical Chemistry

Event Hall THU 11:00~13:00

Structural dynamics study of push-pull chromophores during the intramolecular charge transfer

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Department of Chemistry, Gwangju Institute of Science and Technology, Korea
[1]*Gwangju Institute of Science and Technology, Korea*

Intramolecular charge transfer (ICT) has been of great interest in chemistry and related fields as one of the fundamental chemical reactions. Many experimental and theoretical studies including time-dependent density functional theory (TDDFT) simulations have suggested the structural changes of push-pull chromophores during the ICT process including twisted molecular geometry of the electron-donating or accepting group. But, these investigations have focused on the experimental absorption and emission spectra not vibrational spectra of chromophores, so there is a limit to understanding the structural information during the ICT. Recently, we reported the twisted ICT of 4-dicyanomethylene-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM) with a rotation of electron-donating dimethylamino group by femtosecond stimulated Raman spectroscopy with both high spectral ($^{-1}$) and temporal (

Poster Presentation : **PHYS.P-172**

Physical Chemistry

Event Hall THU 11:00~13:00

2D Mxene/$BaTiO_3$@g-C_3N_4 nanosheets as z-scheme photocatalyst for efficient dye degradation

Jishu Rawal, Soo-Jin Park[1,*]

CHEMISTRY AND CHEMICAL ENGINEERING, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

Novel Z-scheme based heterojunction of graphitic carbon nitride/Ti_3C_2 MXene/ $BaTiO_3$ (CN/MX/BT, CXB) was synthesized via calcination synthesis. Moreover, same composite with graphene as a replacement of MXene was synthesized for comparison of 2-D material effect on the $BaTiO_3$@g-C_3N_4 photocatalytic activity. Comparatively most suitable nanocomposite has achieved high photodegradation efficiency (> 99 %) of pollutant dye under visible light irradiation within 180 min. The effect of CXB was reflected in the design of Z-scheme heterojunction and bang gap tuning, which were beneficial to form stable heterojunction and improve visible light absorption range with faster carrier transfer and stronger redox ability. Moreover, the mechanisms of dye degradation over Z-scheme heterojunction CXB were elucidated.

Poster Presentation : **PHYS.P-173**

Physical Chemistry

Event Hall THU 11:00~13:00

Excited-State Aromaticity of [26]- and [26]- Diazahexaphyrins and Electron Delocalization Effect

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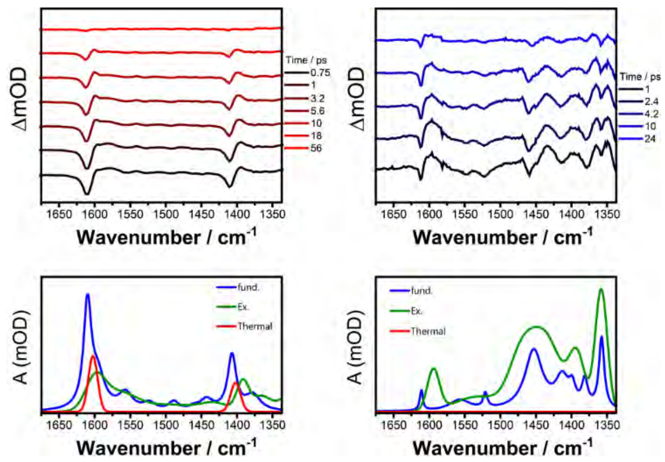
[1]*Department of Chemistry, Yonsei University, Korea*

Expanded porphyrins with hetero-atom at meso-positions provide a fresh concept of aromaticity, arising from the unique contribution from their lone pair electrons in the π-conjugation. Understanding the origin of aromaticity and the excited state behaviors of the expanded meso-heteroporphyrins are important to enlightening the design of novel classes of heteroporphyrin-based functional materials for practical application of the optoelectronic devices. The diazahexaphyrins are reported to show distinct aromaticity switching by redox reactions with maintenance of dumbbell-like conformations and the same π-conjugation pathways. Based on the flexible and adaptable electronic networks on the dumbbell conformations via lone-pair electrons of nitrogen, we investigated the excited state aromaticity through using visible pump and visible-NIR and IR probes. The diazahexaphyrins shows reversed electronic absorption features in the excited state regarding to their aromaticity. Also in the transient IR spectra, [26]- and [28]-diazahexaphyrins showed interconvertible IR spectra with those of counterparts in the ground-state, with the structural effects by hydrogen bonding. The electron delocalization factors extracted through the quantum calculations methods showed distinct different features, representing the contribution of the lone-pair electrons with same π-conjugation networks.


ΔmOD
Time / ps
0.75
1
3.2
5.6
10
18
56
Time / ps
1
2.4
4.2
10
24
1650 1600 1550 1500 1450 1400 1350
Wavenumber / cm^{-1}
A (mOD)
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Thermal

Poster Presentation : **PHYS.P-174**

Physical Chemistry

Event Hall THU 11:00~13:00

Preparation of Mxene assisted BiO_2 heterostructure with enhanced photocatalytic activity and stability

Jishu Rawal, Soo-Jin Park[1,*]

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[1]*Department of Chemistry, Inha University, Korea*

MXene assisted BiO_2 nanocomposites are synthesized via two processes i.e. hydrothermal process and calcination process. Two method of preparation are used to determine the well suited synthesis scheme for the enhanced photocatalytic activity with highly active and well homogenized end product. Moreover, different percentages of MXene as a sensitizer is used to rationalize the nanocomposite composition. The morphology, crystal structure, optical spectroscopy, visible light photocatalytic activity, and photoelectrochemical activity are systematically analyzed and discussed. Incorporation Ti_3C_2 nanosheets into BiO_2 plates has widen up the absorption region. Whereas, interface between Ti_3C_2/BiO_2 accelerates the charge separation and transfer of electrons. Thus, obtained Ti_3C_2/BiO_2 nanocomposites attributes to the improved dye degradation as compared with pure BiO_2. Finally, active species role is determined and photocatalytic mechanism is proposed.

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Event Hall THU 11:00~13:00

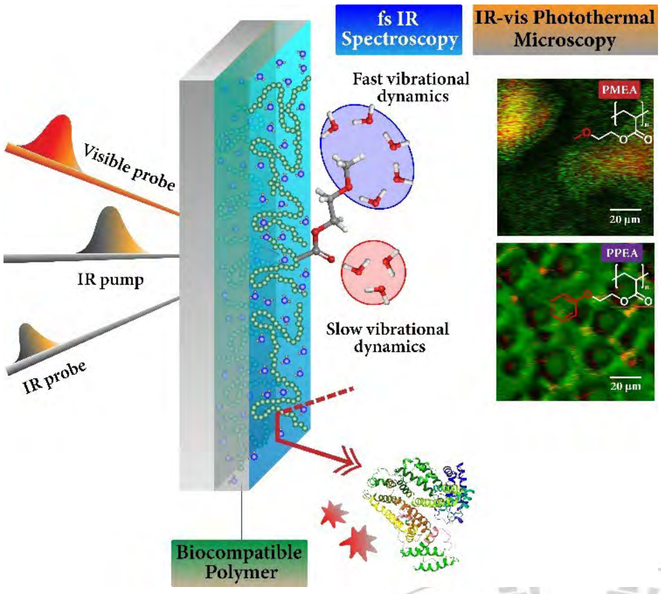
Role of Adsorbed Water on the Biocompatibility of the Acrylate-based Polymers

Saptarsi Mondal, Kyungwon Kwak[1,*], Minhaeng Cho[1,*]

Chemistry, Korea University, Korea

[1]*Department of Chemistry, Korea University, Korea*

The role of water in the excellent biocompatibility of the acrylate-based polymers widely used for anti-biofouling coating material has been realized previously. Here, we report femtosecond mid-infrared pump−probe spectroscopy of the OD stretch band of HOD molecule adsorbed on highly biocompatible poly(2-methoxyethyl) acrylate [PMEA] and poorly biocompatible poly(2-phenoxyethyl) acrylate [PPEA], both of which reveal that there are two water species with significantly different vibrational lifetime. PMEA interacts more strongly with water than PPEA through the H-bonding interaction between carbonyl (C=O) and water. The vibrational lifetime of the OD stretch in PPEA is notably longer by factors of 3 and 7 than those in PMEA and bulk water, respectively. The IR-pump visible-probe photothermal imaging further unravels substantial spatial overlap between polymer CO group and water for hydrated PMEA and a significant difference in surface morphology than those in PPEA. Furthermore, anisotropic relaxation dynamics of the CN stretch mode of PhSeCN molecule embedded inside the polymer matrix unravel the underlying relationships of polymers’ free volume element size, probability distribution, and topography fluctuation dynamics with the water permeability and biocompatibility.


fs IR Spectroscopy
IR-vis Photothermal Microscopy
Fast vibrational dynamics
Slow vibrational dynamics
Visible probe
IR pump
IR probe
PMEA
PPEA
20 μm
20 μm
Biocompatible Polymer

Poster Presentation : **PHYS.P-176**

Physical Chemistry

Event Hall THU 11:00~13:00

Optical Property of the PbSe Colloidal Quantum Dots near 10 μm

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Korea University, Korea

[1]*Department of Chemistry, Korea University, Korea*

The colloidal quantum dots with the steady-state intraband transition has attracted a lot of attention since they allow access to smaller energy than bandgap energy in nanomaterials. So far, the steady-state intraband transitions of Ag_2Se, HgSe, and β-HgS CQDs have been successfully demonstrated in previous research by changing the stoichiometry and surface condition of the nanocrystal. Here, we demonstrate the optical property of PbSe CQDs in the mid-infrared region without post-synthesis. By adjusting the amount of ligand and temperature, the intraband transition emerges near 10 μm, which is manifested in the Fourier transform infrared (FT-IR) spectrum. Furthermore, Photoluminescence (PL) spectroscopy, X-ray photoelectron spectroscopy and, spectroelectrochemistry were conducted to thoroughly examine the origin of the mid-IR absorption feature.

Poster Presentation : **PHYS.P-177**

Physical Chemistry

Event Hall THU 11:00~13:00

Development of a MATLAB Algorithm for Calculating Reorganization Energy of Bridged Dimer System Utilizing the Concept of Local Charge State Fixation

Hyeok Yun, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

To calculate the electron (or hole) hopping reorganization energy in a dimer system in which the donor and acceptor are bridged by molecule, the geometry and force constants of the system in which the charge is localized in the donor or acceptor are required. However, since these states are not ground states, the optimization process is difficult. We developed a local charge state fixation (LCSF) method to calculate the reorganization energy required for the hopping of electron (or hole) in molecule-bridged silicon quantum dot (Si QD) dimer systems. Local charge state fixation refers to a method of replacing a donor (or acceptor) of a neutral state dimer with a donor (or acceptor) of a charged state monomer. In this process, the internal geometry and force constants of the charged state donor (or acceptor) are fixed and grafted. Geometry optimization and force constant matrix calculation of neutral state dimers and charged state donor and acceptor were performed in the Gaussian 16 package. We adopt DFT/B3LYP method and 6-31G(d,p) basis set. Matrices generation of grafted systems was implemented on MATLAB. Reorganization energies between grafted systems were calculated through normal mode analysis. Si QDs with a diameter of 0.83 nm ($Si_{35}H_{35}$) were used for donor and acceptor. And polyethylene (PE), polyacetylene (PA), oligoyne (OY), p-divinylbenzene (VPV), 1,2-Bis(4-vinylphenyl)ethyne (VPEPV), 1,4-bis(4-ethenylphenylethynyl)benzene (VPEPEPV) were used for bridging molecule.

Poster Presentation : **PHYS.P-178**

Physical Chemistry

Event Hall THU 11:00~13:00

Calculation of Electron Transport Properties in π-Conjugated Molecule-Bridged Si QD Dimer Systems By Electron Injection into the Conduction Band of Si QDs

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[1]*Department of Chemistry, Chonnam National University, Korea*

Silicon is a promising material for lithium-ion battery (LIB) anodes due to its high specific capacity. A silicon quantum dot (Si QD) cluster in which Si QDs are connected by π-conjugated molecules has several advantages. First, the electron coupling of Si QDs increases. In addition, the separation of Si QDs is prevented even if the volume changes due to Li^+ ion charging and discharging. These characteristics are thought to enable the performance improvement of LIB. We calculated the electron transport properties of the π-conjugated molecule-bridged Si QD dimer system using the NEGF method to investigate the electron transport of Si QD clusters. When the LIB is charged or discharged, electrons move through the conduction band of the Si QDs. Therefore, it is necessary to obtain the electron transport characteristics considering the electron flow of the LIB anode material. The electron transport properties were calculated by integrating the transmission function through the conduction band. The injected electrons were defined by integrating DOS from the fermi level until the number of electrons equals 2. This calculation was performed according to the length of π-conjugated chains: vinyl-phenyl-vinyl (VPV), vinyl-phenyl-ethynyl-phenyl-vinyl (VPEPV), vinyl-phenyl-ethynyl-phenyl-ethynyl-phenyl-vinyl (VPEPEPV).

Poster Presentation : **PHYS.P-179**

Physical Chemistry

Event Hall THU 11:00~13:00

Calculation of Electron Transport Properties of π-conjugated molecules using small Au cluster with artifically continous DOS in NEGF method

Jiyoung Bang, **Hyun-Dam Jeong**[1,*]

Department of chemistry, Chonnam National University, Korea

[1]*Department of Chemistry, Chonnam National University, Korea*

Non-equilibrium Green's function (NEGF) method can simulate electronic transport through a molecule between metal electrodes, which is affected by the density of states (DOS) of electrodes as well as the molecules. In order to reduce the influence of the electrodes, a bulk metallic electrode with an almost constant DOS below the Fermi level is required. However, it is very difficult to implement the bulk electrode. This is because, as the electrode size increases, the computational cost required for optimization increases exponentially. So, we propose a method to mimic the bulk electrode by using the Au cluster electrode with the same structure as the tip of the gold bulk electrode. Replacing the Fock matrix of the bulk gold electrode tip with that of Au clusters makes the DOS of the Au cluster electrodes smoother, similar to the DOS of the bulk. We obtained linear I–V curves from a system of electrodes connected by 1D Au wires. This means that our proposed method behaves like bulk. The systems were optimized in Gaussian16W and the NEGF method was performed in MATLAB.

Poster Presentation : **PHYS.P-180**
Physical Chemistry
Event Hall THU 11:00~13:00

Improving V-Dock: Design of novel drug-like molecules using docking socre of predictive model based on machine-learning and molecular optimization

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[1]*Department of Chemistry, Kangwon National University, Korea*

In this study, molecular docking and machine learning algorithms were used to design molecules with high binding affinity with desired target. Through the molecular docking program, binding affinity for the target was predicted and learned by the generation algorithm, combinatorial optimization-based algorithm, MolFinder. Finally, the purpose of this study is to create optimal molecules with high QED values and desired properties that can actually be synthesized. At this time, this study can be said to be reliable assuming that the docking score, which quantifies the binding affinity between the target and the molecule through the molecular docking program, actually predicts the activity of the target. Thus, we benchmarked three docking programs: Auto-dock gpu, Openeye, and Glide. We used these three docking programs to dock lit-pcba dataser to test if each docking score could actually classify between active ligands and inactive ligands. Also, we tested whether predictive models trained with these data could classify them. Among the docking programs, docking through Glide was the most reliable. For that reason, Molfinder was trained through a docking score through a glide to generate molecules with desired properties. We believe that our results will open new possibilities for ML- assisted molecular design.

Poster Presentation : **PHYS.P-181**
Physical Chemistry
Event Hall THU 11:00~13:00

Calculation of Dissociative Electron Attachment Reaction Accessibility of Dialkyltin Dicarboxylate Molecules

Hyeok Yun, Hyun-Dam Jeong*

Department of Chemistry, Chonnam National University, Korea

We calculated dissociative electron attachment (DEA) reaction accessibility to estimate the sensitivity of dialkyltin dicarboxylate-based extreme ultraviolet (EUV) photoresists. The DEA reaction is a reaction in which low-energy electrons collide with a molecule (**A**) and dissociate into an anion fragment ($\mathbf{B}^{-}$) and a radical fragment ($\mathbf{C}^{\bullet}$). The DEA reaction accessibility is a value of how well a molecule can be dissociated in the form of an expected structure in the DEA process. The DEA reaction accessibility can be calculated from the mth unoccupied molecular orbital of **A** ($\mathbf{\Psi^{(m)}_{A}}$) and its energy ($\mathbf{E^{(m)}_{A}}$), the nth unoccupied molecular orbital of $\mathbf{B}^{\bullet}$ ($\mathbf{\Psi^{(n)}_{B^{\bullet}}}$) and its energy ($\mathbf{E^{(n)}_{B^{\bullet}}}$), and the total energy of **A** ($\mathbf{E_{A}}$), $\mathbf{B}^{\bullet}$ ($\mathbf{E_{B^{\bullet}}}$) and $\mathbf{C}^{\bullet}$ ($\mathbf{E_{C^{\bullet}}}$). Optimized structures and MO coefficients of **A**, $\mathbf{B}^{\bullet}$, and $\mathbf{C}^{\bullet}$ were calculated in the Gaussian 16 package. We adopt MP2 method and CEP-121G basis set. It was confirmed that the accessibilities are in good agreement with experimental results measured sensitivities of dialkyltin dicarboxylate series.

Poster Presentation : **PHYS.P-182**

Physical Chemistry

Event Hall THU 11:00~13:00

Electronic Structure of Indium Oxide Nanocrystal Thin Film Based on Cyclic Voltammetry and Energy-resolved Electrochemical Impedance Spectroscopy

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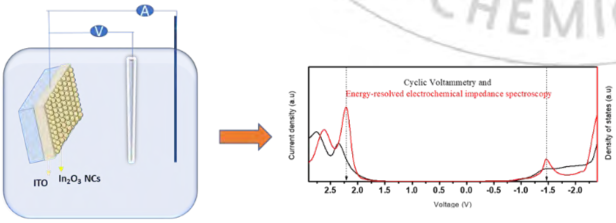
Chonnam National University, Vietnam

[1]*Department of Chemistry, Chonnam National University, Korea*

We demonstrate cyclic voltammetry (CV) and energy-resolved electrochemical impedance spectroscopy (ER-EIS) as quick methods to quantify the electronic structure in nanocrystal thin films. The electrodes for ER-EIS and CV measurements were fabricated by spin-coating with a solution of In2O3 nanocrystal (In2O3 NC) capped with oleic acid (OA), benzoic acid (BA), and 4-aminobenzoic acid (4ABA) on an ITO substrate, then cured at 150, 200, and 250 °C. According to the results, the bandgap of In2O3 NC-based thin films increased as the organic ligand length increased and decreased as annealing temperature increased. In addition, the electronic coupling between the neighboring nanocrystals in BA−capped In2O3 NC and 4ABA−capped In2O3 NC thin films was determined based on Marcus' theory.



Poster Presentation : **PHYS.P-183**

Physical Chemistry

Event Hall THU 11:00~13:00

Calculation of Phonon Transport through Organic Molecule Bridges in Silicon Quantum Dot Dimer Using Atomistic Green's Function Method

Hyeok Yun, Hyun-Dam Jeong[*]

Department of Chemistry, Chonnam National University, Korea

We calculated the thermal conductivity of various kinds of molecule bridge in silicon quantum dot (Si QD) dimer systems with atomistic Green's function (AGF) method in various temperatures (T=0 K~1000 K). Polyethylene (PE), polyacetylene (PA), oligoyne (OY), p-divinylbenzene (VPV), 1,2-bis(4-vinylphenyl)ethyne (VPEPV), 1,4-bis(4-ethenylphenylethynyl)-benzene (VPEPEPV) were selected for the molecular bridges. Si QDs with a diameter of 0.83 nm ($Si_{35}H_{35}$) were used for contacts. Geometry optimization and force constant matrix calculation of the Si QD dimer systems were performed in the Gaussian 16 package. We adopt DFT/B3LYP method and 6-31G(d,p) basis set. The AGF method was implemented on MATLAB R2018b code. Thermal conductivities of the PA bridge systems were, for the most part, the lowest. We suggest using PA as a molecular bridge to increase thermoelectric performance when making thermoelectric materials with Si QD.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

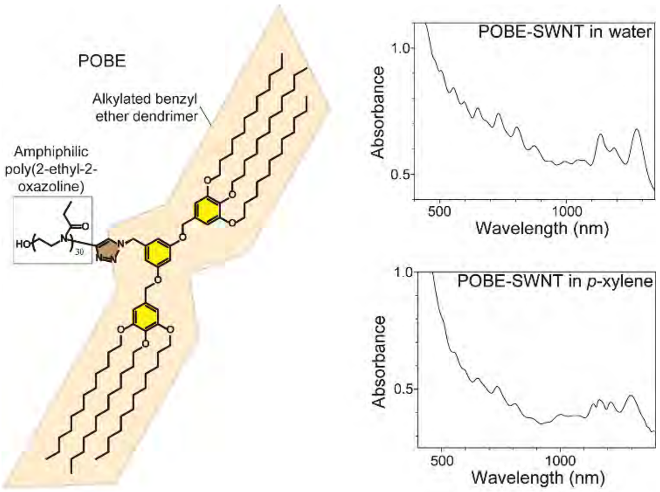
Event Hall THU 11:00~13:00

Diameter separation of Carbon Nanotube using Amphiphilic Poly(2-ethyloxazoline) Derivative

Seokhyeon Son, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Single-walled carbon nanotubes (SWNTs) have unique properties that depend on their chirality, called a pair of integers (*n*, *m*). Due to the heterogeneity of SWNTs, it is important to separate the chirality. Among the various SWNT separation methods, the aqueous two-phase extraction method based on poly(ethylene oxide)/dextran has a simple experimental procedure and low cost. However, this method relies on the gradual replacement of the two surfactants, which provides relative hydrophilicity to the two aqueous phases upon replacement of the surfactants, leading to chiral separation. This requires multiple extraction steps to differentiate the chemical potential difference between the SWNT chirality when replacing the two surfactants.In this poster, we found that amphiphilic polymer surfactants not only disperse SWNTs into aqueous and organic phases, but also separate the chirality of SWNTs according to SWNT diameter (d_t) when mixing the two dispersions. For this purpose, poly(2-ethyl oxazoline)-alkylated second-generation benzyl ether (POBE) was used as a universal surfactant for both aqueous and organic phases. In addition, large partitioning of POBE-SWNTs is facilitated by the phase transfer catalyst, tetrabutylammonium bromide (TBAB). Quantitatively determine d_t-selective extraction by obtaining absorption spectroscopy-based partition constants, K(concentration of SWNTs in organic/concentration of SWNTs in aqueous phase). Efforts are currently being made to increase the number of K to create a clean phase and interface and repeat extraction experiments.


POBE
Alkylated benzyl ether dendrimer
Amphiphilic poly(2-ethyl-2-oxazoline)
HO
N
O
30
N
N
N
O
O
O
O
O
O
O
POBE-SWNT in water
Absorbance
1.0
0.5
500
1000
Wavelength (nm)
POBE-SWNT in p-xylene
Absorbance
1.0
0.5
500
1000
Wavelength (nm)

Poster Presentation : **PHYS.P-185**

Physical Chemistry

Event Hall THU 11:00~13:00

Electrocatalytic nitrite reduction over Cu@Cu2O core-shell with tailored architectures by pulsed laser for sustainable ammonia production

Sang Hun Yeon, Theerthagiri Jayaraman[1], Jiwon Kim, Yiseul Yu, Seung Jun Lee[1], Myong Yong Choi[1,*]

Gyeongsang National University, Korea

[1]*Department of Chemistry, Gyeongsang National University, Korea*

Nitrite produced from industrial and agricultural processes has imbalanced the global nitrogen cycle. The presence of high nitrite (NO2-) concentration in natural water constitutes a serious issue to the environment and human health. Electrocatalytic reduction is a sustainable route to remediate nitrite while generating product of ammonia. Therefore, the development of low-cost, stable non-precious metal catalysts is imminent for efficient NO2- reduction. Herein, we synthesized Cu@Cu2O core-shell architectures by pulsed laser ablation in water as solvent. The intrinsic physicochemical properties of the produced Cu@Cu2O core-shell was analyzed using UV-vis, X-ray diffractometer, Raman, field emission scanning electron microscopy, and transmission electron microscopy. The origin of the prominent activity enhancement for Cu@Cu2O core-shell toward selective nitrite electroreduction to ammonia was systematically investigated. Indo-phenol absorption method was performed to quantify ammonia. This study demonstrates a new architype for designing the stable and cost-effective electrocatalyst for NO2- reduction.

Poster Presentation : **PHYS.P-186**

Physical Chemistry

Event Hall THU 11:00~13:00

The anisotropic circular dichroism of jet-cooled mandelic acid and its hydrated cluster

Jiyeon Yun, Changseop Jeong, Nam Joon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

The electronic circular dichroism (CD) spectra of mandelic acid (MA) and its mono-hydrated cluster ($MA(H_2O)_1$) in a supersonic jet were investigated using dual-beam resonant two-photon ionization circular dichroism (R2PICD) spectroscopy. The IR-UV double resonance spectrum showed that MA was present as a single conformer in the jet. The R2PICD spectrum of MA near the origin band of the S_0-S_1 transition exhibited well-resolved vibronic CD band. The R2PICD spectra of $MA(H_2O)_1$ were also obtained to investigate hydration effects on the CD values of bare MA.

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Poster Presentation : **PHYS.P-187**
Physical Chemistry
Event Hall THU 11:00~13:00

Surface Analytical Studies on Organic Materials using Laser and QIT-ToF-SIMS

Chang Min Choi

Center for Scientific Instrumentation, Korea Basic Science Institute, Korea

Over the past few decades, time-of-flight secondary ion mass spectrometry (ToF-SIMS) with various cluster ion beam apparatuses has been used a powerful instrument for a surface analysis and chemical imaging. Especially the coupling ToF-SIMS with gas cluster ion beams (GCIBs) help us to observe secondary molecular ions from a sample surface for image analysis of biological samples including tissues and cells. Even though it has great advantages, simple ToF mass spectra often have a difficulty assigning a peak which might exist candidates having a similar mass. Recently, some ToF-SIMS developers have been trying to add tandem mass spectrometric function.Therefore, a quadrupole ion trap time-of-flight secondary ion mass spectrometer (QIT-ToF-SIMS) has been developing to resolve the aforementioned problem. Secondary ions are generated from a sample surface with 20 keV toluene ion projectile produced by a UV pulse. The sputtered ions are transferred to a QIT though an extraction electrode and a set of electrostatic lens. After ion accumulation in QIT, the stored waveform inverse Fourier transform (SWIFT) pulse are applied to the QIT for the selection of an interested molecular ion. A laser pulse is irradiated onto the selected secondary ion in the QIT for the photo-induced dissociation (PID). The PID-resulting ions are detected by ToF-MS. The electronic absorption probability is obtained by recording photodepletion of the secondary molecular ion as a function of the laser wavelength.In this study, different molecular ions with similar mass are separated by photodepletion spectra. This would help us eliminate candidates with a confusion come from a similar mass. And furthermore, we anticipate PID study for a secondary ion open a chance to see a surface in a new perspective.

Poster Presentation : **PHYS.P-188**

Physical Chemistry

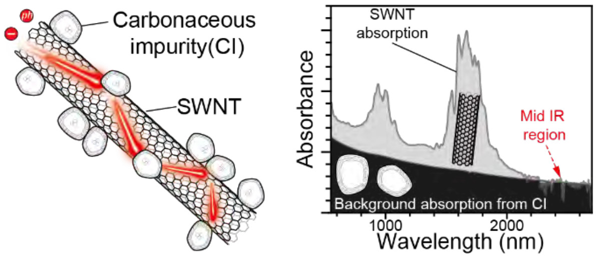
Event Hall THU 11:00~13:00

Quantification and Removal of the Carbonaceous Impurity in a Single-walled Carbon Nanotube Dispersion *via* UV-vis-MWIR Absorption Background

Minsuk Park, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Carbonaceous impurity (CI) is the by-products during the growth process of single-walled carbon nanotube (SWNT). CI affects on the optoelectronic properties as well as on the ability to use absorption spectroscopy to estimate the metallic content of a SWNT dispersion. Therefore, accurate quantification and removal method of CI is required. In this presentation, we have devised methods to characterize and quantify the CI present in SWNT dispersions and to determine the effects of CI on the optical, electrical, and thermal properties of SWNT. A technique to quantitatively determining CI from the finding that chloroform selectively disperses CI presents in SWNT batch. CI separated by dispersing as-purchased SWNT in chloroform has the morphology of agglomerated few-layered graphenes whose size and location depend on SWNT batches. Moreover, CI exhibits UV-vis-mid-wavelength IR (MWIR) absorption curve and an extinction coefficient comparable to graphene. The MWIR absorption region, which possess least absorptions caused by transitions of various SWNT types, was utilized to assess the significant contribution made by CI present in a SWNT dispersion. In addition, a study comparing the chloroform-based CI extraction method with the typically used oxidative purification method showed that the former produces more highly purified SWNT not containing much oxidative damage. Finally, we found that CI present in a SWNT dispersion more strongly lowers thermal conductivity than it does electrical conductivity of a SWNT film. The results of this study provide a way to understand the negative effects that CI has on the optoelectronic properties of SWNT as well as the beneficial effects of excluding ubiquitous CI in SWNT.


ph
Carbonaceous impurity(CI)
SWNT
SWNT absorption
Mid IR region
Background absorption from CI
Absorbance
1000
2000
Wavelength (nm)

Poster Presentation : **PHYS.P-189**

Physical Chemistry

Event Hall THU 11:00~13:00

Efficient hydrazine oxidation of AuPt Alloys Using Integrated Pulsed Laser Irradiation

Yiseul Yu, Seung Jun Lee, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Replacing the kinetically sluggish anodic oxygen evolution reaction (OER) with hydrazine (N2H4) oxidation reaction (HzOR) could be the effective approach for achieving energy-saving hydrogen (H2) fuel production in a water electrolyzer system. Thus, developing the efficient HzOR electrocatalysts, combined with the cathodic H2 evolution reaction (HER) is of vital importance for the high-rate H2 fuel generation as well as for the advancement of a N2H4 fuel cell. Herein, we utilized a facile integrated process of pulsed laser irradiation and sonochemical process to synthesize AuPt alloys by the irradiation of laser to a mixture of Au/Pt solution in methanol/DI water in varied proportions. The AuPt alloy plays a key role in the chemisorption of N2H4 on its surface, forming a dative bond involving electrons of the lone pair of nitrogen in N2H4 and empty orbitals of Pt in the alloy, indicating its high intrinsic activity against HzOR. The optimal composition of Au1Pt8 electrode demonstrates outstanding characteristics of HER with an ultralow overpotential of 26 mV at 10 mA cm−2 in alkaline medium while requiring 502 mV to attain 10 mA cm−2 for HzOR in 0.5 M N2H4/1.0 M KOH electrolyte. In addition, the assembled overall N2H4 splitting electrolyzer cell using Au1Pt8 alloys as both anode and cathode requires cell voltage of only ~0.172 V at 10 mA cm−2 with tremendous stability over 10 h, which is much lower than the voltage of 1.773 V required for the overall water splitting electrolyzer. The present study validates the feasibility of AuPt alloys for stimulating N2H4 fuel cells in the future to achieve both electrical energy generation and high-rate H2 fuel production.

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Poster Presentation : **PHYS.P-190**

Physical Chemistry

Event Hall THU 11:00~13:00

Enhanced cancer imaging using glucosamine-conjugated poly-acrylic acid-coated ultrasmall gadolinium oxide nanoparticles in magnetic resonance imaging

Shuwen Liu, Gang Ho Lee[1,*]

Department of Chemistry, Kyungpook National University, China
[1]*Department of Chemistry, Kyungpook National University, Korea*

Owing to a higher demand for glucosamine (GlcN) in metabolic processes in cancer cells than in normal cells (i.e., GlcN effects), cancer imaging in magnetic resonance imaging (MRI) can be highly improved using GlcN-conjugated MRI contrast agents. Here, GlcN was conjugated with polyacrylic acid (PAA)-coated ultrasmall gadolinium oxide nanoparticles (UGONs) (davg = 1.76 nm). Higher positive (brighter or T_1) contrast enhancements at various organs including cancer were observed in human brain glioma (U87MG) tumor-bearing mice after the intravenous injection of GlcN-PAA-UGONs into their tail vein, compared with those obtained with PAA-UGONs as control, which were rapidly excreted through the bladder. Importantly, the contrast enhancements of the GlcN-PAA-UGONs with respect to those of the PAA-UGONs were the highest in the tumor site owing to GlcN effects. These results demonstrated that GlcN-PAA-UGONs can serve as excellent T_1 MRI contrast agents in cancer imaging via GlcN effects.

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Poster Presentation : **PHYS.P-191**

Physical Chemistry

Event Hall THU 11:00~13:00

Applications of commercial optical gratings as mirrors for matter waves

Lee Yeong Kim, Do Won Kang[1], Wieland Schöllkopf[2], Bum Suk Zhao[3,*]

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Mirrors for atoms and molecules could open new frontiers in matter-wave optics with neutral particles. However, the realization of such components has required sophisticated electromagnetic fields, nano-fabrication, or particle cooling because of inherently short de Broglie wavelengths of atoms and molecules and their strong interaction with a surface. We demonstrate that blazed gratings designed for light waves can work as mirrors for atoms and molecules of thermal energy with up to 47% reflectivity when used under grazing incident conditions. The matter-waves of He atoms are reflected from blazed gratings of different periods (20, 3.33, and 0.417 μm) that are commercially available. The specular reflection probability is well described by the multiple edge- diffraction reflection (MEDR) model. When a wave scatters off an array of half-planes at grazing incidence, it undergoes multiple diffractions by the half-plane edges. Within the MEDR model the reflection probability increases with decreasing incidence angle and grating period. This allows us to observe reflection of fragile He clusters (He_2 and He_3) with the 417-nm-period grating, which implies that the grating mirror based on the MEDR mechanism can also work for other exotic particles, such as antihydrogen atoms. It will be possible to prepare an almost perfect mirror (close to 100% reflectivity) for a neutral particle by tailoring the edges of a grating and shortening its period. Our experiment and analysis show that commercial optical blazed gratings can serve as a mirror in matter-wave optics, which paves the way toward developing various matter-wave-optical instruments.

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Event Hall THU 11:00~13:00

X-Ray Attenuation Properties of Ultra-small Platinum Nanoparticles Coated with Three Different Kinds of Ligand as a High-Performance CT Contrast Agent

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[1]*Department of Chemistry, Kyungpook National University, Korea*

Ultrasmall heavy metal synthesis and characterization of highly crystalline platinum nanoparticles coated with three kinds of polymers Poly(acrylic acid) (PAA) (average M_w = ~1800 Da), Poly(acrylic acid-co-maleic acid) (PAAMA) (average M_w = ~3,000 Da), Poly(methyl vinyl ether-alt-maleic acid) (PMVEMA) (average M_w = ~216,000 Da). The observed particle diameter distribution, with (d_{avg} = 1.84 nm an a_{avg} = 10.40 nm) , (d_{avg} = 1.87 nm an a_{avg} = 20.49 nm), and (d_{avg} = 2.05 nm an a_{avg} = 37.49 nm) for PAA, PAAMA, and PMVEMA-coated platinum nanoparticles, respectively. Ligands were strongly bonded to the surface of the suspension sample of platinum nanoparticles through multiple coordination bonds between its numerous carboxyl groups and numerous Pt^{4+} on the nanoparticle surface, which led to exhibited excellent colloidal stability and biocompatibility. Furthermore, the cells treated with ligands coated ultrasmall platinum nanoparticles with the aqueous solution, were nearly non-toxic were good (>75%) up to 20 μM of [Pt]. The x-ray attenuation power of the solution sample was extremely high, likely owing to the contribution of platinum to x-ray attenuation. Platinum x-ray attenuation was ~58% stronger than that of the commercial iodine contrast agent Ultravist at the same atomic concentration, and~200% times stronger than that of Ultravist at the same number density. These findings indicate that the platinum nanoparticle may be a potential CT contrast agent.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

Event Hall THU 11:00~13:00

Synthesis and characterizations of polyacrylic acid coated $YEuO_3$ nanoparticles

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[1]*Department of Chemistry, Kyungpook National University, Korea*

Lanthanide and rare-earth nanoparticles have recently received widespread interest in biological applications. Especially, much attention has been given to the development of luminescent lanthanide nanoparticles for fluorescence imaging (FI) that has high sensitivity and resolution. Among the luminescent lanthanide nanoparticles, the europium-based NPs are better candidates for the imaging application. In the present work, the europium doped yttrium oxides were synthesized via a simple polyol method and coated with polyacrylic acid (PAA) (average Mw=~1800Da) [$YEuO_3$@PAA] to make them water soluble and biocompatible. These nanoparticles showed a red emission at 616 nm corresponding to $^5D_0$-$^7F_2$ forced electric dipole transition of Eu^{3+} ions under UV excitation. Moreover, the europium ions provide effective Stokes shifts, narrow band width, and stable luminescence. These properties make the synthesized nanoparticles useful for fluorescence imaging.

Poster Presentation : **PHYS.P-194**

Physical Chemistry

Event Hall THU 11:00~13:00

Synthesis and Characterization of Ultrasmall Dextran-Coated Gd_2O_3 Nanoparticles as T_1 MRI Contrast Agent

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Department of Chemistry, Kyungpook National University, China

[1]*Department of Chemistry, Kyungpook National University, Korea*

Ultrasmall dextran-coated (M_r=1500 amu) gadolinium oxide (Gd_2O_3) nanoparticles were synthesized utilizing the one-pot synthesis method and their T_1 MRI potential to become excellent T_1 MRI contrast agents was also studied further. The obtained ultrasmall dextran-coated Gd_2O_3 nanoparticles possess good water solubility, originating from an average particle diameter of 1.5 nm and an average hydrodynamic diameter of 12.4 nm, and non-toxicity which was confirmed by a cellular cytotoxicity test. The longitudinal (r_1) and transverse (r_2) relaxivities were tested to be 12.2 and 29.3 $s^{-1}mM^{-1}$ (r_2/r_1=2.4), respectively, much better than those of commonly commercial Gd-chelates. Additionally, the obtained r_1 value is also better than those of published large dextran-coated Gd_2O_3 NPs with an average particle diameter larger than 20 nm. The strengthened T_1 MRI images were observed after injecting obtained sample solution at the mouse tail, exemplifying that the designed ultrasmall dextran-coated Gd_2O_3 NPs own the potential to act as medical T_1 MRI contrast agents.

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Poster Presentation : **PHYS.P-195**

Physical Chemistry

Event Hall THU 11:00~13:00

A Synthetic Method of Ultrasmall Gadolinium Oxides Nanoparticles as Multifunctional MRI agents

Son-Long Ho, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

Herein, we report the synthesis of poly(acrylic acid) conjugated with Rhodamine and further coated on ultrasmall gadolinium oxides nanoparticles. These nanoparticles were applied later as MRI contrast agent and thank to Rhodamine moiety, these nanoparticles can be used to differentiate cancer and normal cells, since the cancer cells possess lower pH level than normal cell.Moreover, we applied these nanoparticles in in vitro gadolinium neutron capture therapy against U87MG cell line and the result showed a higher cell death rate compare to commercially available MRI contrast agent Gadovist.

Poster Presentation : **PHYS.P-196**

Physical Chemistry

Event Hall THU 11:00~13:00

Polyaspartic acid-coated gadolinium oxide nanoparticles were synthesized for T_1 and T_2 magnetic resonance imaging

Huan Yue, Gang Ho Lee[1,*]

Department of Chemistry, Kyungpook National University, China

[1]*Department of Chemistry, Kyungpook National University, Korea*

The relaxometric properties of the nanoparticles are affected by the surface coating polymers because they contribute to nanoparticle based magnetic resonance imaging contrast agents. In this research, polyaspartic acid coated ultrasmall gadolinium oxide (PASA-Gd_2O_3) nanoparticles were synthesized through by one-pot polyol method. The average diameter was estimated to be 2.0 nm. A significant longitudinal (r_1) and transverse (r_2) water proton spin relaxivity with value of 19.1 and 53.7 $s^{-1}mM^{-1}$, respectively, (r_2/r_1=2.8) under a 3.0 tesla MR field which is approximately 5 and 10 times higher than those of commercial Gd-chelate molecular contrast agents, respectively. indicating their potential as a dual-modal T_1 and T_2 MRI contrast agent.

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Event Hall THU 11:00~13:00

Various ligand-coated ultrasmall gadolinium-oxide nanoparticles: effect of ligand-Size and ligand-chain hydrophilicity on spin relaxation

Tirusew Tegafaw, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

In this study, we report Ligand-size and ligand-chain hydrophilicity effects on the relaxometric properties of ultrasmall Gd_2O_3 nanoparticles. The ligands used for the coating include small diacids with hydrophobic chains, namely, succinic, glutaric acid, and terephthalic acid and large polyethylenimines (PEIs) with hydrophilic chains, namely, PEI-1300 (M_n=1300) and PEI-10000 (M_n=10000). The particle diameter was monodisperse with an average value of 1.3 nm. The structural, morphological, surface coating, toxicity and their water proton relaxation were explained based on the magnetic dipole interaction between the dipoles of the nanoparticle and water proton.

Poster Presentation : **PHYS.P-198**

Physical Chemistry

Event Hall THU 11:00~13:00

Poly (methyl vinyl ether-alt-maleic acid)-coated Gadolinium Oxide Nanoparticles for T_1 MRI Contrast Agents

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In nanomedicine, surface modification of nanoparticles is important because nanoparticles should have good colloidal stability and biocompatibility. In this respect, the surface coating of the material plays an important role, and hydrophilic ligands capable of providing high colloidal stability are preferred for the surface coating. Importantly, it can give high r_1 values as it allows many water molecules to access gadolinium oxide nanoparticles (Gd_2O_3 NPs). Therefore, various surface coating materials should be studied and coated. In this study Poly(methyl vinyl ether-alt-maleic acid) PMVEMA-coated Gd_2O_3 NPs with ultrasmall particle size distributions (davg = 1.9 nm) were synthesized using one-pot polyol synthesis. PMVEMA-coated Gd_2O_3 NPs showed good colloidal stability in water and good biocompatibility in cellular toxicity tests. The r_1 relaxivity value of 36.3 $s^{-1}mM^{-1}$, which is approximately ten times higher than those of commercial contrast agents. This high r_1 value was attributed to large hydration diameters of the PMVEMA-coated Gd_2O_3 NPs (aavg=18.6 nm). The effectiveness of the PMVEMA-coated Gd_2O_3 NPs was demonstrated by taking in vivo T_1 MR Images in mice. Strong positive contrast enhancements were observed in T_1 MR images after intravenous administration of the solution sample into mice tails, demonstrating that PMVEMA-coated Gd_2O_3 NPs act as a T_1 MRI contrast agents.

Poster Presentation : **PHYS.P-199**

Physical Chemistry

Event Hall THU 11:00~13:00

Circular dichroism spectroscopy of jet-cooled (S)-(–)- and (R)-(+)-styrene oxide

Seon gyeong U, Seo Yeong Jeong, Jiyeon Yun, Changseop Jeong, Nam Joon Kim*

Department of Chemistry, Chungbuk National University, Korea

The circular dichroism (CD) spectra of chiral molecules in solution display averaged CD values of all conformational isomers in solution. However, the CD spectra of cold, isolated molecules provide conformation-selective CD values. Here, we investigate the electronic CD spectra of (S)-(–)- and (R)-(+)-styrene oxide produced in a supersonic jet using dual-beam resonant two-photon ionization CD (R2PICD) spectroscopy. The IR ion-dip spectra reveal that the styrene oxide exists as a single conformer in the jet. The R2PICD spectra exhibit different shapes of CD bands for different vibronic bands. We discuss the effect of a vibrational mode on the shape of a CD band.

Poster Presentation : **PHYS.P-200**

Physical Chemistry

Event Hall THU 11:00~13:00

Rational Design Engineering Structure of Ir doped NiMoP/CNTs Heterostructure Supported by CNT-Graphene for Overall Water Splitting

Hien Van Hoa, Do hwan Kim[1,*]

나노융합공학과, Jeonbuk National University, Korea

[1]*Department of Chemistry Education, Jeonbuk National University, Korea*

Rationally designing efficient and robust catalysts with cost-effective and high-performance electrocatalysts for bifunctional water splitting have been exploring in industrial H2 produce to replace fossil fuel. In this study, doping Ir atoms into both phase of an amorphous NiMoPxOy and crystalline of NiMoP phase generates enriched active sites with high intrinsic activity, the catalyst material coating on the CNTs-Gr/Cu foam (CF) serves as an electron transport pathway, improve surface area and protective layer (Ir-(NiMoP-NiMoPxOy)/CNTs-Gr/CF). The designed material has outstanding electrochemical water splitting properties, the optimized Ir-(NiMoP-MoNiPxOy)/CNTs-Gr shows with a tiny overpotential of 90 mV at 10 mA cm-2 for the hydrogen evolution reaction and 220 mV at 20 mA cm-2 for the oxygen evolution reaction. Long-term stability of Ir-(NiMoP-NiMoPxOy)/CNTs-Gr/CF in 1.0 M KOH is demonstrated by a cell voltage of 1.72 V at 50 mA cm-2 after 150 hours, indicating a retention of 90%. Our result suggests an attractive electrocatalyst with low cost and high catalytic activity for bifunctional water splitting. This research was supported by the Regional Leading Research Center Program (2019R1A5A8080326) through the National Research Foundation funded by the Ministry of Science and ICT of the Republic of Korea.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Event Hall THU 11:00~13:00

Vibration-mediated valence to non-valence state transition in the ground state of isolated anion

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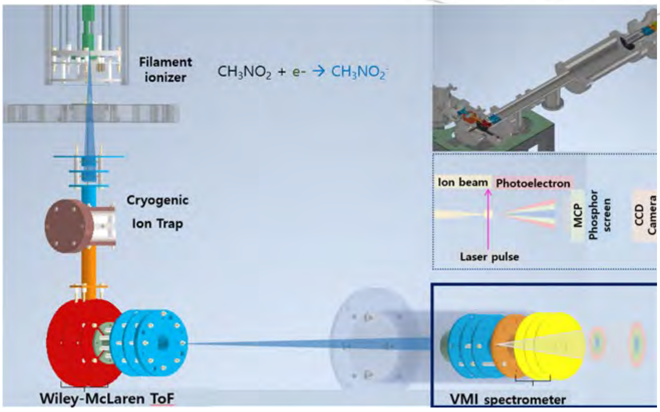
The first observation of electron transfer between the valence to non-valence orbital by the vibrational energy is presented. Dipole-bound state (DBS), one of the non-valence states, is observed after the vibrational excitation with the picosecond-IR laser pulse. A newly constructed cryogenic open-shell anion photoelectron spectrometer was used to observe the valence to non-valence dynamics of the nitromethane anion. By tuning wavelength, we also found out DBS formation yield is maximized when photon energy is resonant to the vibrational frequency of the valence-bound state(VBS), giving new insight into the role of the vibration in the coupling between VBS and DBS. Surprisingly, we also observed that the direct photoemission process forms the DBS, which implies that the photodetached electron is recaptured by the DBS. Our experimental observations regarding electron capturing capability and vibronic coupling mechanism of the DBS support that the non-valence state is a doorway state of electron attachment reaction



Poster Presentation : **PHYS.P-202**

Physical Chemistry

Event Hall THU 11:00~13:00

Prediction of a supersolid phase in high-pressure deuterium using isobaric-isothermal Boson path integral molecular dynamics

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Supersolid is a mysterious and puzzling state of matter whose possible existence has stirred a vigorous debate among physicists for over 60 years [1]. Its elusive nature stems from the coexistence of two seemingly contradicting properties, long-range order and superfluidity [2]. We report computational evidence of a supersolid phase of deuterium under high pressure ($p > 800$ GPa) and low temperature ($T < 1.0$ K)[3]. In our simulations, that are based on bosonic path integral molecular dynamics[4] and machine learning potential[5], we observe a highly concerted exchange of atoms while the system preserves its crystalline order. The exchange processes are favoured by the soft-core interactions between deuterium atoms that form a densely packed metallic solid. At the zero-temperature limit, Bose-Einstein condensation is observed as the permutation probability of N deuterium atoms approaches 1/N with a finite superfluid fraction. Our study provides concrete evidence for the existence of a supersolid phase in high-pressure deuterium and could provide insights on the future investigation of supersolid phases in real materials[6].References[1] E. Kim and M. H. Chan, Nature (London) 427, 225 (2004).[2] D. Thouless, Ann. Phys. (N.Y.) 52, 403 (1969).[3] C. W. Myung, B. Hirshberg, M. Parrinello, Phys. Rev. Lett. Accepted (2022)[4] B. Hirshberg, V. Rizzi, M. Parrinello, Proc. Natl. Acad. Sci. U.S.A. 116, 21445 (2019).[5] J. Behler and M. Parrinello, Phys. Rev. Lett. 98, 146401 (2007).[6] P. Loubeyre, F. Occelli, P. Dumas, Nature (London) 577, 631 (2020).

Poster Presentation : **PHYS.P-203**

Physical Chemistry

Event Hall THU 11:00~13:00

The peroxynitrous acid generation via the reaction between nitrous acid and hydrogen peroxide in the ice grain boundary

Yong Yoon Ahn, Kitae Kim*

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Peroxynitrous acid is a non-selective oxidizing reagent as well as nitration reagent. To produce peroxynitrous acid via the reaction of hydrogen peroxide and nitrous acid, the acidic condition is required because the reaction between hydrogen peroxide and nitrite is quite slow and the speciation of nitrite to nitrous acid require the acidic condition (pKa (HNO_2/NO_2^-) = 3.2). In this study, we suggested that the freezing hydrogen peroxide and nitrite mixture at mild acidic condition (above pH 4) accelerates the generation of peroxynitrous acid by pH degrease at the ice grain boundary due to the freezing concentration effect of protons. The generation of peroxynitrous acid was confirmed by the chemical transformation of benzoic acid. The characteristic of the reaction was investigated through monitoring the benzoic acid degradation in varying parameters, such as initial pH, dosage ratio, and functional group on the benzoic acid. The detection of the byproducts of benzoic acid transformation using the ultrahigh-performance liquid chromatography/electrospray ionization/mass spectrometry system (UHPLC/ESI/MS) also conducted to study the reaction of peroxynitrous acid. As freezing is a global phenomenon, and hydrogen peroxide and nitrite are ubiquitous in the environment, the transformation of aromatic compounds with H_2O_2/NO_2^- in cold area need to be under the consideration.

Poster Presentation : **PHYS.P-204**

Physical Chemistry

Event Hall THU 11:00~13:00

Automated Design of Synthesizable Molecules Using Structure-Conditioned Generative Model

Juhwan Noh, Dae-Woong Jeong[1], Kiyoung Kim[2], Se-Hui Han[3], Moontae Lee[4], Yousung Jung[*]

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[1]*LG AI Research, Korea*
[2]*LG AI research, Korea*
[3]*Materials Informatics Lab, LG AI Research, Korea*
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Design of molecules with target functionality is an ultimate goal in various applications including drugs, photovoltaic, OLED and so on. But, the conventional trial-and-error-based approaches are resource demanding, and thus many data-driven chemical researches are proposed to accelerate new discoveries. Deep generative models combined with molecular big database have particularly attracted a significant attention in recent years since they could effectively learn the continuous embedding of molecules. While the trained latent representation is useful tool to design molecules with optimal properties, only tiny fraction of the generated molecules is experimentally synthesized and validated its functionality. Thus, predicting synthesizability or retrosynthetic planning have been proposed as post-hoc analysis tools, but those processes could be slow and ineffective. In this talk, therefore, I will present a generative model that generates both molecules and their reaction routes that are analogous of the target motif structures. Our benchmark shows ability to generate structure- and property-wise similar molecules, and also to further improve chemical activity of the given seed molecules under the awareness of reaction routes.

Poster Presentation : **PHYS.P-205**

Physical Chemistry

Event Hall THU 11:00~13:00

Lasing of axial-heterostructure AlGaN/GaN/InGaN nanorods

Sangwon Nam, Sunghyun Jung, Jae Kyu Song*

Department of Chemistry, Kyung Hee University, Korea

One-dimensional semiconductor nanolasers are expected for photonic, optoelectronic, and electronic applications. The axial-heterostructure nanorods of AlGaN/GaN/InGaN are promising candidates for building blocks for optoelectronics, because they have distinct band structures and waveguiding properties. We investigate the optical properties of multiple-layered axial-heterostructure nanorods composed of AlGaN/GaN/InGaN and observe polariton lasing of GaN for the first time. The lasing of nanorods can be controlled by modulation of the gain volume, layer sequence, and end facet.

Poster Presentation : **PHYS.P-206**

Physical Chemistry

Event Hall THU 11:00~13:00

Effect of Secondary Structure on the Membrane Disruption of Antimicrobial Peptides in Bacterial Cell Membranes: A Molecular Dynamics Simulation Approach

Inhyeok Choi, Yeonho Song, Hyonseok Hwang*

Department of Chemistry, Kangwon National University, Korea

Antimicrobial peptides (AMPs) are a class of small peptides that play a crucial role in the host defense system against invading pathogens such as bacteria. These peptides display amphiphilic properties that have both positively charged and hydrophobic residues. In this study, we used molecular dynamics (MD) simulations and potential of mean force (PMF) calculations to assess the importance of α–helical properties of AMPs and the interaction of AMPs with Gram-negative bacterial cell membranes composed of POPE and POPG lipid molecules. To investigate the effect of secondary structure on the insertion of AMPs into the bacterial cell membrane, we used two types of AMPs: LK and LK-L8P. LK is composed of leucine(L) and lycine residues and LK-L8P is a modified LK with leucine at position 8 replaced by proline(P). Our MD simulations and PMF calculations show that LK maintains stable α-helical structures both inside and outside the membrane and features a double-well type free energy variations. In contrast, the α-helical secondary structure of LK-L8P is not retained very well due to proline residue. In addition, only a single free energy minimum is found inside the membrane for LK-L8P, indicating that LK-L8P penetrates more easily into the membrane than LK.

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April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-207**

Physical Chemistry

Event Hall THU 11:00~13:00

Proton migration in amorphous ice at cryogenic temperatures

Du Hyeong Lee[*], **Heon Kang**[1]

Korea Polar Research Institute, Korea
[1] *Department of Chemistry, Seoul National University, Korea*

Proton hopping in ices is well known for Grotthuss mechanism, but it has been hardly observed at cryogenic temperatures using experimental methods. Accordingly, in this study, we measured the proton migration distances in ice at both 10 K and 80 K to study the proton hopping mechanism to study the temperature dependence of the migration. The proton transfer efficiency was determined by the generated ammonium ions after accepting protons from hydrogen chloride molecules, and the distance was calculated by integrating the efficiency as a function of the distance between the proton donor (HCl) and the acceptor (NH3). The average migration distance of protons at 10 K and 80 K did not show a considerable difference. This result indicates that the proton transfer at cryogenic temperatures occurs via proton hopping, a quantum tunneling process, which is hindered by defects in the hydrogen bond network.

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April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **PHYS.P-208**

Physical Chemistry

Event Hall THU 11:00~13:00

Photocatalytic dehydrogenation of cis-1,4-cyclohexanediamine on Pd- and Au-deposited TiO_2(110) surface

Jeong Su Kang, Hyung-Joon Shin[1,*]

Materials Science Engineering, Ulsan National Institute of Science and Technology, Korea
[1]*School of Materials Science and Enginnering, Ulsan National Institute of Science and Technology, Korea*

Hydrogen can be stored in a liquid organic hydrogen carrier (LOHC) in a form of chemical bond with carbon. We can stably store or release the hydrogen gas by forming or breaking these bonds in LOHC molecules. Most of recently studied LOHC molecules rely their hydrogen storage ability on the cyclohexane-benzene transformation. However, it is hard to break the C-H bond of cyclohexane therefore requires catalysts and high temperature. In this study, we investigated the photocatalytic dehydrogenation of cis-1,4-cyclohexanediamine on Pd- and Au-deposited rutile TiO_2(110) single crystal surface by low-temperature scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). The photocatalytic dissociation of C-H bond by 365 nm wavelength UV irradiation is observed on the Pd- and Au-deposited TiO_2, but not on the bare TiO_2 surface. We showed the metal-induced change in the electronic structure on TiO_2(110) surface and suggested that the reaction is induced by the hot electrons, produced by the dielectric response of the TiO_2(110) against the plasmonic metal nanoparticles.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Event Hall THU 11:00~13:00

Effect of Nanoparticle Materials and Shapes on Hot Carrier Generation

Ly Thi Minh Huynh, Seokheon Kim, Sangwoon Yoon*

Department of Chemistry, Chung-Ang University, Korea

Hot electron chemistry is of paramount significance because of its applicability to photocatalytic reactions, solar energy conversion, and waste decomposition. The nonradiative decay of excited plasmons in gold or silver nanoparticles generates highly energetic nonthermal electrons and holes (namely, hot carriers) that can induce chemical reactions when transferred to nearby molecules. Among many decay mechanisms, electron-surface scattering plays a major role in the formation of hot carriers. Therefore, the hot carrier generation efficiency must sensitively depend on the characteristics of nanoparticles. In this poster, we present our recent experimental studies to measure the effect of nanoparticle material type, and shape on the hot carrier generation efficiency. These findings will contribute to the design of highly efficient plasmonic photocatalysts and photovoltaic devices.

Poster Presentation : **PHYS.P-210**

Physical Chemistry

Event Hall THU 11:00~13:00

Chitosan-EDTA modified magnetic biochar for removal of radioactive cobalt(II) from aqueous solutions

Park Bogyeong, Sangjun Choi[1,*]

School of Architectural, Civil, Environmental, and Energy Engineering, Kyungpook National University, Korea

[1]*Department of Environmental Engineering, Kyungpook National University, Korea*

Magnetic biochar functionalized with chitosan and EDTA(Ethylenediaminetetraacetic acid) composite(CMBC-EDTA) was synthesized for efficient and economic, and eco-friendly removal of radionuclide Co^{2+} in aqueous solution. To examined its physical and chemical properties, elemental analyzer, surface area & pore size analyzer, Fourier-transform infrared spectroscopy, field emission scanning electron microscope auto-thermogravimetric analyzer, X-Ray Diffractometer, X-Ray photoelectron spectroscopy and vibrating sample magnetometer were used. The removal efficiency of Co^{2+} was analyzed by inductively coupled plasma optical emission spectroscopy. In the isotherm studies, CMBC-EDTA was well fitted to Langmuir model (R^2=0.9951) better than Freundlich model (R^2=0.9335). According to Langmuir model, it has a Co^{2+} maximum adsorption capacity of 22.49 mg/g. Also, in the kinetic studies, it reached adsorption equilibrium very quickly. Co^{2+} uptake occurs well the wide range pH except lower than pH2 where the adsorption capacity falls sharply. The magnetization intensity of CBMC-EDTA was 19.416 emu/g which is enough to magnetic separation and reuse.

Poster Presentation : **PHYS.P-211**

Physical Chemistry

Event Hall THU 11:00~13:00

Removal of arsenic using a graphene oxide magnetic adsorbent impregnated to black tea tannin

Min young Lee, **Sangjun Choi**[1,*]

School of Architectural, Civil, Environmental, and Energy Engineering, Kyungpook National University, Korea

[1]*Department of Environmental Engineering , Kyungpook National University, Korea*

Arsenic, which is mainly exposed to the human body through drinking water, causes various changes in the body, causing cancer and cardiovascular diseases in vivo, and in addition, skin diseases, respiratory diseases, and Neurological diseases are reported. We need adsorbent material that can remove such arsenic effectively and ecofriendly. Black tea is an eco-friendly adsorbent material that contains a large amount of tannin, a type of polyphenol. Black tea tannin (BT) has the chelating ability supported by abundant adjacent materials, showing excellent ability to remove heavy metal cations. The tannin fraction was separated from the black tea extract by Sepadex LH-20 column chromatography using ethanol and 50% (v/v) acetone. And the content was calculated using the vanillin analysis method to obtain a value of 52 mg/g. This is a very high content compared to other plants. However, pure tannin is dissolved well in water and unstable, so heavy metal arsenic was removed by synthesis of mag@GO@BT. mag@GO@BT adsorbent was characterized by a physicochemical method, and showed excellent adsorption capacity at 303 K and pH 7 with a maximum adsorption capacity of 2.120 mg/g. The adsorption process of arsenic followed the Langmuir isotherm model and kinetic equation. All experimental results show that adsorbent mag@GO@BT has good adsorption ability to remove arsenic, and adsorbent has good magnetic force, making it easy to separate and reuse.

Poster Presentation : **PHYS.P-212**

Physical Chemistry

Event Hall THU 11:00~13:00

[Withdrawal] UVC Photo-Fenton Decomposition behavior of oxalic Waste depending on H_2O_2 and iron catalyst concentration.

Saifur Rahman, **Dohyeon Kim**[1], **Sangjun Choi**[1,*]

School of Architectural, Civil, Bangladesh

[1]*Department of Environmental Engineering, Kyungpook National University, Korea*

- Withdrawal -

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Event Hall THU 11:00~13:00

Machine learning models for predicting the experimental frontier orbital energies

Minseok Jeong, Gahyun Lee, Minhi Han, Sungnam Park[1,*]

Chemistry, Korea University, Korea
[1]*Department of Chemistry, Korea University, Korea*

The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies are key factors in optoelectronic devices and must be accurately estimated for newly designed materials. Recently, machine learning methods based on the quantum calculation databases have emerged as a promising solution to predict molecular properties with substantially reduced computational costs. However, these models have several limitations to be practically used in material development because quantum calculation databases contain relatively small molecules and do not include molecule-environment interactions which significantly affect molecular properties. In this work, to overcome the aforementioned limitations, we have constructed an experimental database of HOMO and LUMO energies measured under different experimental conditions and methods and we have investigated several machine learning models using various molecular representations. The performances of the machine learning models will be discussed and compared.

Poster Presentation : **PHYS.P-214**

Physical Chemistry

Event Hall THU 11:00~13:00

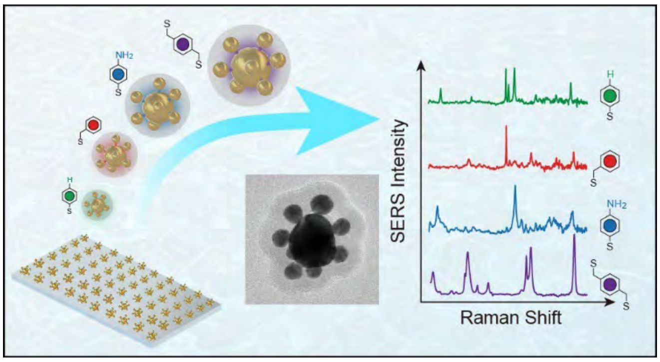
Silica-Encapsulated Core–Satellite Gold Nanoparticle Assemblies as Stable, Sensitive, and Multiplex SERS Probes

Hoa Duc Trinh, Sangwoon Yoon[1,*]

Chemistry, Chung-Ang University, Korea

[1]*Department of Chemistry, Chung-Ang University, Korea*

Developing highly sensitive and stable surface-enhanced Raman scattering (SERS) probe systems is an actively pursued goal in sensors and diagnostics. In this study, we present silica-coated core-satellite ($CS@SiO_2$) plasmonic nanoparticle assembly structures that potentially realize this goal. We assemble different-sized gold nanoparticles into core-satellite (CS) configurations using dithiol molecular linkers that also serve as SERS labels. Multiple hot spots in the CS structure and narrow nanogaps in each hot spot produce a significantly enhanced Raman scattering signal with an enhancement factor of ~8×10^7. Various types of molecules can be inserted into the nanogaps using the mixed self-assembled monolayers with alkanedithiol, enabling multiplex detection. Silica encapsulation of the CS nanoassemblies stabilizes the particles and makes it easy to modify the surface to attach antibodies or DNAs. Many properties of the $CS@SiO_2$, including a wide range of optical resonances, scalability using multiple glass slides, long-term stability in ethanol, and single-particle-level sensitivity, make the material an ideal SERS probe for sensitive and multiplexed detection of diseases and viruses.



Poster Presentation : **PHYS.P-215**

Physical Chemistry

Event Hall THU 11:00~13:00

Methology of MoS_2-$MoSe_2$ core-shell heterosucture transition metal dichalcogenides synthesis

Insu Lim, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Transition metal dichalcogenides(TMD) have semiconductor properties. Depending on the combination of transition metal and chalcogen, the bandgap can be small up to 1.0-2.5 eV and various photoelectric characteristics can be exhibited, thereby attracting attention as a next generation semiconductor material. Among them, heterostructure of TMD can give wide attention to the physics and technology of new devices by controlling the optical and electronic properties of transition metal dichalcogenides.This poster describes the synthesis of heterostructure of TMD, which are lateral MoS_2-$MoSe_2$ core-shell, using chemical vapor deposition. In order to form TMD having a lateral heterostructure, MoS_2 was first synthesized on a silicon substrate, and then a chalcogen precursor was changed into Se to grow crystal grains mixed with MoS_2, $MoSe_2$, and MoSSe. The synthesis was carried out in an Ar and H_2 atmosphere, and it was confirmed by Raman and optical microscopy that MoS_2, $MoSe_2$, and MoSSe crystal grains grew. After that, it can be observed that S and Se were shown in the form of an alloy with a heterostructure of TMD, and the fluorescence spectrum occurring at this time was changed in accordance with the ratio of S and Se. Growth conditions of different structures of two-dimensional materials capable of implementing various semiconductor energy structures according to a combination of materials may be optimized, and band gap control and fluorescence absorption control may be easily performed, thereby manufacturing various types of various types of optoelectronic devices.

Poster Presentation : **PHYS.P-216**

Physical Chemistry

Event Hall THU 11:00~13:00

Compressively Strained Transition Metal Dichalcogenide Dispersions Using van der Waals Heterostructure Strategy

Sungmin Bong, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Although various methods have been developed to disperse transition metal dichalcogenides (TMDCs) in aqueous solution, a strategy to disperse stable TMDC still remains a great challenge. In this experiment, I would like to introduce a strategy to disperse the TMDC wrapped structure with hexagonal boron nitride(hBN) and sodium cholate (SC). In TMDC dispersion with hBN and SC, changes in excitons due to compressive strain caused by the presence of hBN and SC can be observed through extinction spectrum. Unlike TMDC in an intrinsic state, a blue shift can be seen in a dispersed solution, and this difference contrasts with a phenomenon not seen in TMD synthesized by general chemical vapor deposition. The colloidal stability of dispersion could be confirmed through zeta potential measurement. In general, when the absolute value is greater than 30 meV, colloidal dispersion can be said to be stable, and since the TMDCs measured in this experiment have values between -41.4 and -52.0 mV, it can be confirmed that stable colloidal is formed. As a result of confirming the size of these colloidal through a transmission electron microscope, it was confirmed that they had a hydrophobic layer with a defect with a flake size of several hundred nm^2. Through Raman spectroscopy, it was possible to confirm the effect of hBN on TMDC according to centrifugal force. As the *g* force increased, the blue shift of E^1_{2g} and A_{1g} could be confirmed, which could further explain the existence of compressive strain

Poster Presentation : **PHYS.P-217**

Physical Chemistry

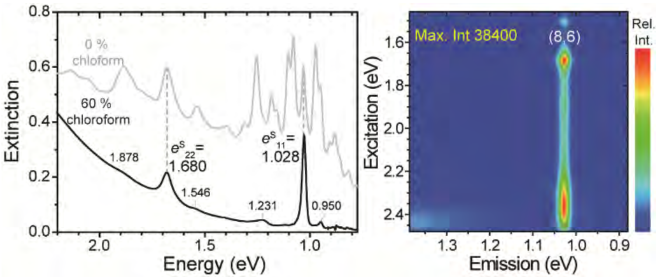
Event Hall THU 11:00~13:00

Electron-Phonon Interaction in Single Chirality Enriched Single-Walled Carbon Nanotubes Wrapped by Flavin Surfactant

<u>SeongJoo Hwang</u>, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Understanding excited electron and vibration is a pivotal to understand the optoelectronic pathways of single-walled carbon nanotube (SWNT) having unique electronic band structure. In this study, we have studied optical spectrum of a single chirality SWNT that is prepared by dispersion of *N*-dodecyl isoalloxazine (FC12) used as a surfactant and subsequent addition of chloroform to the dispersion. The separated (8,6) tube exhibits that absorption spectrum contains strong first (e_{11}) and second (e_{22}) transitions at 1.028 eV and 1.680 eV, respectively. Moreover, those bands accompanied by broad bands separated from e_{11} and e_{22} by 190 meV to the high energy sides. Those bands are attributed to electron-phonon interaction mainly originating from G and G' bands of Raman modes. In addition, we observed small side band of e_{11} and e_{22} to the lower energy side whose origin is not clear currently. In photoluminescene excitation (PLE) map, those bands are clearly discernable from the optical transitionspeaks with maximum intensity appear at the crosspoint positions of e_{11} and e_{22} as well as the wide excitation by energy transfer from FC12 to e_{11}. FC12 acts as a background in the absorption spectrum, and excitation occurs at 0.973 eV and 2.43 eV in the PLE map. The spectroscopic characteristics of SWNTs derived from FC12 are supported by AFM image of SWNTs uniformly surrounded by FC12 in a helix structure.



Poster Presentation : **PHYS.P-218**

Physical Chemistry

Event Hall THU 11:00~13:00

Study of Selective Crystal Facet of Cu_2O Microcrystal to Improve Photocatalytic Performance

Sung Min Heo, Yong Ho Lee, Chang Woo Kim[1,*]

Department of Smart Green Technology Engineering, Pukyong National University, Korea
[1]*Department of Nanotechnology Engineering, Pukyong National University, Korea*

This study is to increase efficiency by controlling active sites using facet control for photocatalytic characteristics using sunlight. Cu_2O has a narrow band gap (2.1 eV) capable of absorbing light in the visible light region, and each side has a unique surface atomic arrangement, such that stability, light absorption characteristics, chemical selectivity, and reactivity vary. In this study, in a simple experimental method, three types of Cu_2O particles were synthesized: a cube with {100} facet, a cube with {100}/{111} facet, and an octahedral type with {111} facet. During the experiment, Cu_2O particles having various surfaces could be synthesized by controlling the amount of Poly vinyl pyrrolidone(PVP), which is a surfactant. PVP adsorbs on the {111} surface of Cu_2O to suppress growth, thereby exposing the Cu_2O {111} surface. This study plans to increase charge separation efficiency by synthesizing metal organic framework materials with Cu_2O in the future.

Poster Presentation : **PHYS.P-219**

Physical Chemistry

Event Hall THU 11:00~13:00

Physics-informed Deep Learning Framework for Generalizing Drug-target Interaction Prediction

<u>Seokhyun Moon</u>, Wonho Zhung[1], Soojung Yang[2], Woo youn Kim[3,*]

Dept. of Chemistry, Korea Advanced Institute of Science and Technology, Korea

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[2]*Computational and System Biology, Massachusetts Institute of Technology, United States*

[3]*Department of Chemistry, KAIST, Korea*

Recently, deep neural network (DNN)-based drug-target interaction (DTI) models were highlighted for their high accuracy with affordable computational costs. Still, the insufficient generalization for the unseen drug target remains a challenging problem in the practice of computer-aided drug discovery. In this work, we propose two key strategies for better generalization of the DTI prediction with DNN. Primarily, we predict the interatomic interactions between drug and target via physics-informed equations, including learnable parameters, where a structure-based graph neural network is trained to provide the optimal values. These pairwise interactions are then combined to obtain the total binding affinity of the drug-target complex. We further improve the model's generalization ability by adopting a broader range of binding complexes — poses and ligand species — as training data. Our model, named PIGNet, was benchmarked with the comparative assessment of scoring functions (CASF) 2016, demonstrating the outperforming docking and screening powers than previous structure-based approaches. Our physics-informing strategy enables the interpretation of predicted affinities by visualizing the substructure-wise contribution, providing insights for ligand R-group optimization.

Poster Presentation : **PHYS.P-220**

Physical Chemistry

Event Hall THU 11:00~13:00

Exploring extensive chemical space by fragment-based molecular generative model to design *de novo* TADF emitter

Jun Hyeong Kim, Woo youn Kim[1,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, KAIST, Korea*

Thermally activated delayed fluorescence (TADF) emitter is one of the promising organic light-emitting diodes. Various design approaches have been proposed, but conventional design methods rely on human experience and prior design knowledge, resulting in a few fragments and combinatorial rules. Likewise, high-throughput virtual screening can overcome previous limitations of adopting a large library but still suffers from practical issues such as high computational cost. Here, we propose an efficient data-driven approach to search expanded chemical space for novel TADF emitter discovery using the fragment-based molecular generative model. The generative model-based TADF emitter design approach is unnecessary to predefine constraints such as donors, acceptors, and combinational rules; therefore, it can search extensive chemical space. Also, it is efficient because conditional generation produces molecules with the desired properties, resulting in a more focused set of molecules. We show novel TADF emitter candidates can be generated based on the proposed workflow.

Poster Presentation : **PHYS.P-221**

Physical Chemistry

Event Hall THU 11:00~13:00

Spatially Constrained 3D Scaffold-based Molecular Generative Modeling Toward a Controllable Drug Design

Wonho Zhung, Woo youn Kim[1,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemistry, KAIST, Korea*

De novo molecular design has been the subject of immense interest, as it has numerous applications. Remarkably, the scaffold-based generative modeling is highlighted as an effective way of generating desirable molecules where much of the chemical functionalities are preserved by its core structure. In drug discovery, one primary goal is to elaborate the scaffold to increase binding affinity and selectivity toward a binding pocket. Yet, encountering the surrounding 3D geometry of a given pocket remains a challenging problem in previous approaches. In this light, we propose a spatially-constrained 3D scaffold-based generative model. Specifically, we adopted a variational-autoencoder architecture, where the binding structure of a whole molecule is first embedded as a latent vector. The decoder then estimates the probability distributions of types and interatomic distances from the latent vector. Two different distance distributions --- the distance between ligand atoms and the distance between ligand and pocket atoms --- are separately modeled. During the generation, we used an auto-regressive process where the next type and coordinate are sampled from the learned distribution sequentially. As a result, our model can generate valid and diverse molecules from the given pocket and the scaffold. We demonstrated the selectivity of the generated molecules, where the molecule generated from the cognate receptor is barely bound to the non-cognate receptors. Finally, we leveraged the conditional generation scheme to control the properties of generated molecules, providing a possible framework for scaffold optimization.

Poster Presentation : **PHYS.P-222**

Physical Chemistry

Event Hall THU 11:00~13:00

Synthesis and characterization of shape-tunable hexagonal nickel titanate

Yong Ho Lee, Sung Min Heo, Chang Woo Kim[1,*]

Department of Smart Green Technology Engineering, Pukyong National University, Korea
[1]*Department of Nanotechnology Engineering, Pukyong National University, Korea*

Photocatalysts with a band gap to visible light responsive materials has been attracting an attention to improve their efficiency. Among them, $MTiO_3$ (M = Co, Ni, Co etc) materials are attracted widely in the photocatalytic applications due to their optical properties and visible light responsive material. Moreover, research of crystal facet of particles have been attracted substantial attention because their physiochemical characterization is induced by each facet. The induced physiochemical characterization from regular atom arrangement on the surface have a strong impact on the surface reactive reaction. Here, we have demonstrated nickel titanate of hexagonal type morphology, which is synthesized by solvothermal method. Based on solution based approach, morphology of particles was controlled by sodium hydroxide as reducing agent and distilled water concentration. Thus, we obtained the different size of microstructure with hexagonal shape and synthesized plate type particles by controlling the length of the sides of the particles. The morphological and optical properties of synthesized powders were characterized by X-ray diffraction, scanning & transmission electron microscopy, energy-dispersive spectrum and uv-visible spectroscopy.

Poster Presentation : **PHYS.P-223**

Physical Chemistry

Event Hall THU 11:00~13:00

Scoring Synthesizability of Lead-Compounds using Graph-based Machine Learning

Hyeongwoo Kim*, Woo youn Kim[1]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1] *Department of Chemistry, KAIST, Korea*

Recently, thanks to the powerful computational power and improvenment of new techniques, autonomous material design method is being utilized in larger and larger fields. Because material design aims to discover new candidates which are able to be synthesized starting from commercially available chemicals as well as have desired physical and chemical properties, most approaches try to use existing scoring metrics to evaluate the ease of their synthesis. Previous metrics use several information, for instance, how frequently each chemical fragment appears, what chemical reactions are available, and so on. However, those approaches do not consider full-retrosynthetic pathways, they have some lacks of information to evaluate synthesizability of chemicals. In this work, we propose a new evaluation method which can consider retrosynthesis, but still is fast. We have used our method on drug-discovery procedure, and compared with other scoring methods such as SA score and SC score. Lastly, we report a virtual screening experiment result using molecules proposed by several generative models.

Poster Presentation : **PHYS.P-224**

Physical Chemistry

Event Hall THU 11:00~13:00

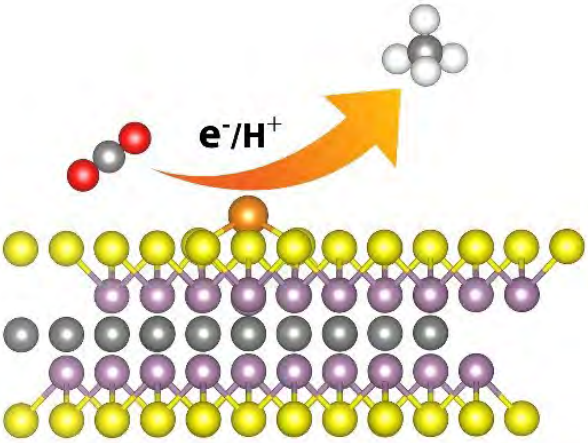
Density functional theory study on the catalytic CO_2 reduction of SACs embedded in S-terminated Mo_2C-MXene

Sambath Baskaran, Jaehoon Jung[1,*]

University of Ulsan, India

[1]Department of Chemistry, University of Ulsan, Korea

Single-atom catalysts (SACs) recently attracted considerable attention in heterogeneous catalysis, owing to high atom-utilization and unique properties. In this paper, we investigated geometry, electronic structure, stabilities, catalytic activity, and selectivity of the various TM@Mo_2CS_2 (TM = Fe, Co, Ni, Cu, Ru. Rh, Pd, Ag, Os, Ir, Pt, and Au) anchored SACs for CO_2 electrochemical reduction using periodic density functional theory and ab-initio molecular dynamics calculations. The single metal atoms tend to occupy the Mo-top site on the Mo_2CS_2 surface. Possible different reaction pathways to produce various C_1 products such as CO, HCOOH, HCHO, CH_3OH, and CH_4 have been investigated for Fe, Co, Ni, and Ru supported SACs. Among the SACs investigated, Fe, Co, and Ru supported by Mo_2CS_2 catalysts selectively produce CH_4, whereas Ru@Mo_2CS_2 has the lowest overpotential of 0.24 eV. Ni primarily produces HCOOH with an overpotential is 0.37 eV. Therefore, this research demonstrated the significant potential of Mo_2CS_2 surface for a single-atom catalyst for selective CO_2 reduction and other electrochemical applications



Single Atom Supported on Mo_2CS_2

Poster Presentation : **PHYS.P-225**

Physical Chemistry

Event Hall THU 11:00~13:00

Competitive excimer formation dynamics of Coumarin dyes anchored on semiconductor films probed by ultrafast time-resolved fluorescence

Yun Jeong Na, Hyunseok Lee, HyungJoo Lee, HyunJae Lee, Chul Hoon Kim*

Department of Advanced Materials Chemistry, Korea University, Korea

Ultrafast interfacial charge injection and excimer formation dynamics of a coumarin dye, 7-hydroxycoumarin-3-corboxylic acid (OHCCA), adsorbed on semiconductor thin films (ZrO2, Al2O3, and TiO2) were systematically investigated by femtosecond time-resolved spectroscopy. OHCCA is structurally robust both in ground and excited states, which allows us to rule out structural relaxation dynamics such as twisted intramolecular charge transfer. In combination of using a co-adsorbent molecule called CDCA, we demonstrated that the interfacial charge injection of OHCCA on TiO2 film does compete with the excimer formation induced by intermolecular interactions. Furthermore, we found that the excited state dynamics of photosensitizer strongly depends on bound structures with the surface of semiconductor. The intrinsic charge injection of the isolated dye on TiO2, which can be prepared with excess CDCA (>1:10000), was determined to be 1 ps. The excimer formation dynamics, however, was gradually modulated with varying the type of semiconductor films: time constants were 940 fs, 550 fs, and 350 fs for ZrO2, Al2O3, and TiO2 films, respectively. That is, the strong orbital interaction between photosensitizing dye and TiO2 surface not only induces the interfacial charge injection, but also deteriorates its efficiency via ultrafast excimer formation. Therefore, the use of co-adsorbents is essential for highly efficient dye-sensitized solar cells based on TiO2.

Poster Presentation : **PHYS.P-226**

Physical Chemistry

Event Hall THU 11:00~13:00

Intramolecular Vibrational Energy Redistribution in Nucleobases: Excitation of NH Stretching Vibrations in Adenine-Uracil+H_2O

Jongbaik Ree[*], Hyung Kyu Shin[1], Yoo Hang Kim[2]

Department of Chemical Education, Chonnam National University, Korea
[1]*Department of Chemistry, University of Nevada, United States*
[2]*Department of Chemistry, Inha University, Korea*

Redistribution of vibrational energy in the adenine-uracil base pair is studied when the base pair undergoes an intermolecular interaction with an overtone-bending vibration excited $H_2O(2\nu_{bend})$ molecule. Energy transfer is calculated using the structural information obtained from density functional theory in the solution of the equations of motion. Intermolecular vibrational energy transfer (VET) from $H_2O(2\nu_{bend})$ to the uracil-NH stretching mode is efficient and rapidly followed by intramolecular vibrational energy redistribution (IVR) resulting from coupling between vibrational modes. An important pathway is IVR carrying energy to the NH-stretching mode of the adenine moiety in a subpicosecond scale, the energy build-up being sigmoidal, when H_2O interacts with the uracil-NH bond. The majority of intermolecular hydrogen bonds between the base pair and H_2O is weakened but unbroken, during the ultrafast energy redistribution period. Lifetimes of intermolecular HB are on the order of 0.5 ps. The efficiency of IVR in the base pair is due to near-resonance between CC and CN vibrations. The condition also facilitates VET between H_2O and NH. When H_2O interacts with the NH bond at the adenine end of the base pair, energy flow in the reverse direction to the uracil-NH stretch is negligible. The energy distributed in the CH bonds is found to be significant, whereas the third hydrogen bond CH…O in the base pair does not significantly affect the overall redistribution. The IVR process is found to be nearly temperature independent between 200-400 K.

Poster Presentation : **PHYS.P-227**

Physical Chemistry

Event Hall THU 11:00~13:00

Solvent Accessibility Measurement of an Intrinsically Disordered Protein by Laser-Assisted NMR spectroscopy

Jonghyuk Im, Jung Ho Lee[1,*]

Department of Chemistry, Seoul National University, Korea

[1]*Division of Chemistry, Seoul National University, Korea*

Intrinsically disordered proteins (IDPs) are abundant in eukaryotes and play important roles in many biological functions. Because IDPs lack well-defined structures, nuclear magnetic resonance (NMR) spectroscopy is well suited to investigate the atomic details of IDPs. Quantitative analysis on solvent accessibility of each amino acid can provide detailed information on conformation. Photochemically induced dynamic nuclear polarization (photo-CIDNP) is laser-assisted NMR spectroscopy and has been used to overcome the low sensitivity limit of NMR spectroscopy. Photo-CIDNP can also be used to measure solvent accessibility of aromatic amino acids in a protein. However, intense laser pulse which is essential for photo-CIDNP experiments often requires a customized NMR spectrometer and its complicated instrumentation has impeded access to its wide usage. Herein, we developed novel instrumentation for photo-CIDNP experiments which does not require customization of NMR spectrometer. NMR pulse sequences were developed to obtain a high-resolution NMR spectrum. Solvent accessibility of aromatic amino acids was measured on an IDP, α-Synuclein, by photo-CIDNP method. Various probes for solvent accessibility measurements were used and their effect was analyzed. Our measurements were extensively validated by comparison with other methods for solvent accessibility measurement.

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Poster Presentation : **ANAL.P-228**

Analytical Chemistry

Event Hall THU 11:00~13:00

Size separation of exosomes and microvesicles by flow field-flow fractionation/multiangle light scattering and the lipidomic comparison

Young Beom Kim, Myeong Hee Moon*

Department of Chemistry, Yonsei University, Korea

Extracellular vesicles (EVs) are lipid membrane particles containing proteins, lipids and RNA species. EVs mediate cell to cell communication and are related to immune signaling, cell differentiation and proliferation. Subpopulations of EVs are divided into exosomes (30-100 nm in diameter) and microvesicles (100-1000 nm) and therefore, it is essential to distinguish them separately because they differ in contents, proteins, and lipid compositions. However, isolation of EVs is still not standardized, and each of the EVs separation methods such as ultracentrifugation, size exclusion chromatography, filtration, and precipitation has its own limitations.In this study, separation of exosomes and microvesicles derived from DU145 cells was demonstrated by frit-inlet asymmetrical flow field-flow fractionation (FIAF4) with UV and multi-angle light scattering (MALS) detectors based on field programming. Fractionated exosomes and microvesicles by Flow FFF were confirmed by western blotting and their sizes were determined by MALS calculation and TEM images. Lastly, lipidomic analysis was performed by nanoflow ultrahigh performance liquid chromatography-electrospray ionization-tandem mass spectrometry to investigate the difference in lipid compositions between exosomes and microvesicles which were collected during the FIAF4 runs.

Poster Presentation : **ANAL.P-229**

Analytical Chemistry

Event Hall THU 11:00~13:00

Lipidomic analysis of different aortic macrophages from hyperlipidemic mice by nanoflow ultrahigh performance liquid chromatography tandem mass spectrometry

Jaewon Seo, Gwang Bin Lee, Myeong Hee Moon*

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Lipidomics is a comprehensive study of lipids including identification and quantification of lipids and lipid metabolism. Lipids, being the major components of cell membranes, play essential biological roles such as cell signaling, energy storage, and etc. Because of lipids' diverse roles in biological systems, their abnormal metabolism has been reported to be linked with several metabolic diseases such as diabetes, obesity, and atherosclerosis. Atherosclerosis is a chronic vascular disease characterized by lipid accumulation and subsequent chronic inflammation of the arterial wall. The rupture of advanced atherosclerotic plaques can eventually lead to heart attack and stroke. Since macrophages play essential role at the initial steps of atherosclerosis by turning into lipid-laden foamy macrophages upon ingestion of excessive LDLs, it is important to investigate lipid perturbations between the foamy and non-foamy macrophages from aortas under atherosclerosis. In this study, lipid profiles of three macrophage populations including intimal foamy and non-foamy macrophages and adventitial macrophages of atherosclerotic mouse aortas were analyzed using nanoflow ultrahigh performance liquid chromatography-tandem mass spectrometry. Only 50,000 macrophages of each group were utilized for the analysis and total of 526 lipids were identified and 187 lipids were quantified. As a result, TGs showed different trends in intimal macrophages according to their chain length, while levels of CEs LPCs, and PEs were found to be significantly higher in foamy macrophages compared to non-foamy macrophages.

Poster Presentation : **ANAL.P-230**

Analytical Chemistry

Event Hall THU 11:00~13:00

Optimization of saliva volume for lipid analysis with nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry

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Saliva is one of the informative biofluids since it contains enzymes, hormones, and lipids that originated from several sources. The biological molecules in saliva are known to be transferred from blood to saliva. Because of this, saliva is known to have a good correlation with serum and plasma and also reflect the physiological status of the body. In addition, saliva has advantages in sampling; easy-to-collect, non-invasive, and painless compared to serum or plasma. For this reason, human saliva gains much interests to be used to develop effective biomarkers for diagnosing, monitoring disease status, and predicting disease progression. Lipids have highly complex structural diversities and play key tools in biological system such as cell signaling and energy metabolism. Despite its potential as a useful biomarker discovery tool, salivay lipid have been poorly investigated yet. Therefore, it is necessary to optimize the lipid extraction method for saliva.In this study, lipid extracts from various saliva volumes (1.0, 0.5, 0.2, and 0.1 mL) were analyzed by nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry (nUHPLC-ESI-MS/MS). The saliva volumes were evaluated by extraction recovery, matrix effect, and the number of quantifiable lipids. The concentration of each lipid class and lipid species was decreased as the saliva volumes were decreased. The number of quantifiable lipids were 221, 241, 158, and 122 at 1.0, 0.5, 0.2, and 0.1 mL of saliva, respectively. As a result of these, the minimum saliva volume was determined to be 0.5 mL which can perform lipidome analysis effectively by nUHPLC-ESI-MS/MS without losing the number of quantifiable lipids.

Poster Presentation : **ANAL.P-231**
Analytical Chemistry
Event Hall THU 11:00~13:00

Flow field-flow fractionation with thickness tapered channel

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Flow field-flow fractionation (FlFFF) is an analytical technique that can separate sample components by sizes with the use of the two flow streams without a stationary phase. Size separation of macromolecules in FlFFF is achieved by the interplay of two perpendicularly moving flows: migration flow (along the channel axis) to transport the sample and crossflow (by the strength of the external field) to retain the sample materials within the channel. Depending on the hydrodynamic diameter, the particles have parabolic flow profiles that are slow near the channel wall and fast at the center. In the steric/hyperlayer mode where particles larger than 1 μm are separated, large particles with higher lift force from the bottom of the channel are located at a faster flow streamline and elute earlier than small particles. Increasing the channel thickness improves the separation efficiency but increased separation time of large particles degrades the sample recovery and resolution. Furthermore, additional flow control equipment and software are required to separate particles in a wide range.In this study, a new type of channel with tapered thickness was introduced to enhance the elution of long retaining sample components in FlFFF. By utilizing a thickness tapered channel, sample migration can be gradually fastened without employing the field programming because the migration flow rate increases along the axis. The separation efficiency of the thickness tapered channel was compared with that of the conventional flat channel by comparing retention time, sample recovery, and steric transition phenomenon under the various flow rate conditions.

Poster Presentation : **ANAL.P-232**

Analytical Chemistry

Event Hall THU 11:00~13:00

Optimization of fecal and saliva sample pretreatment for lipidomic analysis by nanoflow ultrahigh performance-liquid chromatography-electrospray ionization-tandem mass spectrometry

Bo Young Hwang, **Jaewon Seo[1], Gwang Bin Lee[2], Myeong Hee Moon[2,*]**

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[1]*Yonsei University, Korea*
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Lipid profiling for diagnostic purposes has become one of the promising area in relation to metabolomic approach. While most of salivary lipids are originated from serum or plasma, fecal lipids are derived from the gut flora, epithelial cells from the stomach and intestinal tract, and undigested food. Although lipidomic studies about blood and cells have been sufficiently investigated, saliva and fecal lipidomic studies as potential biomarker candidates have not been thoroughly investigated yet.In this study, we have investigated the pretreatment methods of saliva and fecal samples for storage before lipid extraction and the volume of fecal samples needed for lipidomic analysis. Since lipid composition and their levels may change during the transportation between the sampling site and the analytical lab, it is important to investigate the alterations in lipid profile during storage. Saliva samples were exposed in room temperature for 4 days by adding two different types of organic solvents: 95 % EtOH and a mixture of MeOH/MTBE. Lipid profiles of saliva samples treated with organic solvents were evaluated by comparing the normalized peak area of individual lipid species in comparison to that of a fresh saliva sample. Saliva sample mixed with MeOH and MTBE shows the most similar result with the fresh saliva sample than other treatments. Then, Intra Class Correlation (ICC) technique was utilized to verify the degree of maintaining the concentration of lipids in terms of stability and the calculated ICC value was the highest as 0.973 for the saliva treated with MeOH and MTBE condition. In case of fecal samples, the effect of the amount of original feces on lipid identification and quantification was investigated for the optimization, resulting that a. total of 296 lipids were identified from the fecal samples, showing the improvement in lipid identification compared to the reported study.

Poster Presentation : **ANAL.P-233**

Analytical Chemistry

Event Hall THU 11:00~13:00

Liquid chromatography mass spectrometry analysis of urinary metabolites from miscarriage/pre-term cases

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According to Ministry of Health and Welfare of Korea, the rate of birth in Korea has decreased double in 2017 compared to the rate in 2000. A miscarriage is a spontaneous loss of pregnancy before the 20th gestational weeks , and it has been reported that 10-20% of the total pregnancies end in miscarriages. Another pregnancy related problem is a pre-term birth, which is a delivery of infants before 37 weeks of pregnancy. Various reports postulates that the recent decrease in the rate of birth is closely correlated to miscarriage and pre-term birth.Dansyl chloride (DNS-Cl) was utilized to derivatize and enhance the sensitivity of the urinary metabolites from pregnant women. In an effort to discover the potential metabolic biomarkers in the urinary samples from pre-term and miscarriage patients, the relative quantity of metabolites in urine samples from normal pregnancy was compared with those from pre-term and miscarriage patients. DNS-Cl has been widely used as an efficient fluorescence probe for the quantitative analysis of complex molecules with the following functional groups, primary/secondary amines, phenolic, hydroxyl and thiol groups. Recently, DNS-Cl was applied for the derivatization of metabolites and metabolic by-products with amine and phenolic functional groups. Dansylation reaction improves the sensitivity of metabolites and enables the chromatographic separation in reversed-phase mode. Derivatized metabolites were identified and quantified using liquid chromatography tandem mass spectrometry (LC-MS/MS). Retention orders of the derivatized metabolites were investigated from the databases, human metabolome database (HMDB) and MyCompoundID. Six different standard metabolites (L-Arginine, Glycine, L-Proline, L-Phenylalanine, L-lysine, Serotonin) were used to set the relative retention orders of the metabolites in the chromatographic separation. Another set of urinary metabolites were derivatized with 13C-exchanged dansyl chloride and used as an internal standard. By the addition of internal standards in urinary samples from different gestational weeks, the relative quantification of metabolites in urine was carried out. After the relative amounts of urinary metabolites was determined, the amount of creatinine in

each urine sample was used for the normalization. As a result three potential biomarker(Ornithine, Vanillylmandelic acid, Hydroxyphenyllactic acid) were discovered by volcano plot one of the statistical analysis. In the future, consistency of three potential biomarker will be confirmed through additional sample analysis.

Poster Presentation : **ANAL.P-234**

Analytical Chemistry

Event Hall THU 11:00~13:00

Comparison of thermal desorption (TD) sorbent tubes with SPME fibers for the analysis of combustion gases from fossil fuels

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The characterization of combustion gases from fuel oils is important for the identification of cause of fire and investigation of arson suspects. In this study, we combusted three kinds of fuel oils such as diesel, kerosene, and gasoline refined by three different refinery companies, for which combustion gases were characterized using TD/GC-MS and SPME/GC-MS. For the comparison purposes, two TD sorbent tubes (Tenex® TA, and AirtoxTM) and four SPME fibers (PDMS, PDMS/DVB, CAR/PDMS, and DVB/CAR/PDMS) were utilized for gas sampling. The results showed that two different sampling methods have comparable absorption efficiencies. In addition, three different TD sorbent tubes and fibers showed different compatibility to the type of fuel oils. It was found that AirtoxTM, CAR/PDMS, and DVB/CAR/PDMS are suitable for the adsorption of combustion gases from kerosene and diesel. Tenex® TA and CAR/PDMS showed high adsorption compatibility for gasoline. On the other hand, AirtoxTM was found to be the most appropriate adsorption tube for relatively light gases under 130 Da.

Poster Presentation : **ANAL.P-235**

Analytical Chemistry

Event Hall THU 11:00~13:00

Single-Particle Study on Hg Amalgamation Mechanism and Slow Inward Diffusion in Mesoporous Silica-Coated Gold Nanorods without Structural Deformation

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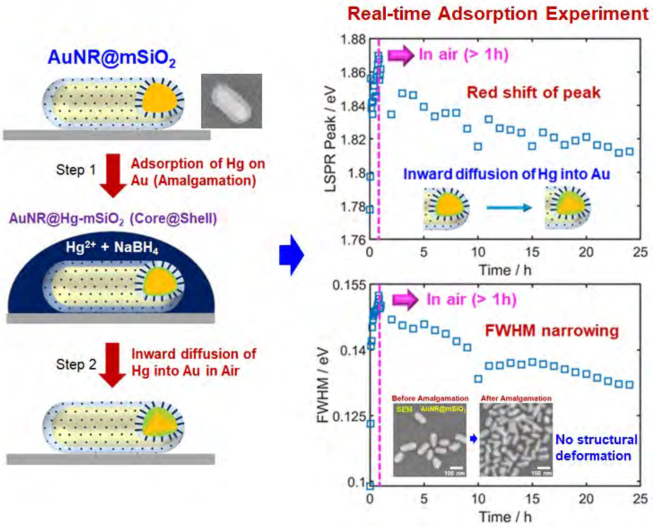
This paper presents the structural and spectral variations of individual mesoporous silica-coated gold nanorods (AuNRs@mSiO_2) compared to bare AuNRs upon Au-Hg amalgamation. First, the aspect ratio of AuNRs@mSiO_2 exposed to Hg solutions was unchanged because the deformation of the AuNR cores was suppressed by the silica shell. Second, dark-field microscopy and spectroscopy revealed a blue shift of the localized surface plasmon resonance (LSPR) wavelength peak and strong plasmon damping in the scattering spectra of individual AuNRs@mSiO_2 exposed to Hg solutions. Furthermore, we investigated time-dependent adsorption kinetics and spectral changes during Au–Hg amalgam formation in single AuNRs@mSiO_2 over a long timeframe. When AuNRs@mSiO_2 were removed from Hg solution, a gradual red shift and linewidth narrowing of the LSPR peak were observed over time due to the inward diffusion of Hg into the AuNR core. Therefore, this study provides new insights into the relationship among amalgamation process, morphological change, role of silica shell, and LSPR peak and linewidth at the single-particle level.


Real-time Adsorption Experiment
AuNR@mSiO$_2$
Step 1
Adsorption of Hg on Au (Amalgamation)
AuNR@Hg-mSiO$_2$ (Core@Shell)
Hg^{2+} + NaBH$_4$
Step 2
Inward diffusion of Hg into Au in Air
In air (> 1h)
Red shift of peak
Inward diffusion of Hg into Au
LSPR Peak / eV
Time / h
In air (> 1h)
FWHM narrowing
Before Amalgamation
After Amalgamation
SEM
No structural deformation
FWHM / eV
Time / h
1.88
1.86
1.84
1.82
1.8
1.78
1.76
0.155
0.14
0.125
0.1
0
5
10
15
20
25

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Poster Presentation : **ANAL.P-236**

Analytical Chemistry

Event Hall THU 11:00~13:00

Nanoceria-based lateral flow immunoassay for hydrogen peroxide-free colorimetric biosensing for C-reactive protein

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During the recent several decades, lateral flow immunoassay (LFIA) constructed with gold nanoparticle (AuNP) has been widely utilized to conveniently detect target analyte. However, AuNP-based LFIA has limitations, such as limited detection sensitivity and quantification capability. Herein, to overcome these constraints, we have developed cerium oxide nanoparticle(nanoceria)-based LFIA for C-reactive protein (CRP) detection in human serum samples. It was fabricated with nanoceria, a notable nanozyme that shows an oxidase activity to quickly oxidize organic substrate, such as 3,3′,5,5′-tetramethylbenzidine(TMB), to produce colored product without any oxidizing agent (e.g., hydrogen peroxide), which is advantageous for realizing point-of-care testing (POCT) applications. By employing human blood serum spiked with CRP, the nanoceria-based LFIA showed two blue-colored lines on the test and control region within 3 min via TMB oxidation, by the captured nanoceria through antigen–antibody interaction. The produced blue-colored lines were distinguished by naked eyes and quantitated with real images acquired by a conventional smartphone with the ImageJ software. With this strategy, target CRP was specifically determined down to 117 ng mL−1 with high detection precisions yielding coefficient of variation of 9.8–11.3% and recovery of 90.7–103.2% using human blood serum samples. This investigation demonstrates the potential of oxidase-like nanoceria for developing LFIA, which is particularly useful in instrumentation-free POCT environments.

Poster Presentation : **ANAL.P-237**

Analytical Chemistry

Event Hall THU 11:00~13:00

Personal passive air sampler development for measuring chlorinated gases from chlorine-based disinfectants

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During the COVID-19 pandemic, chlorine-based disinfectants are being widely used at domestic and public places. However, the misuse of chlorine-based disinfectants can generate high concentrations of harmful gases including chlorine gas. Hence, estimating the exposure level of chlorinated gases while using chlorinated disinfectants is necessary. Here, we developed a personal passive air sampler (PPAS) composed of *o*-dianisidine and a polydimethylsiloxane (PDMS) sheet: *o*-dianisidine which is doped inside the PDMS changes its color due to the oxidation reaction with chlorinated gases. Thus, the PPAS developed in this study allow to detect personal exposure to the chlorinated gases by the naked eyes, while cumulative exposure could be determined by measuring reduced mass of *o*-dianisidine after exposing to the chlorinated gases. By a chamber test, calibration of PPAS was successfully conducted with obtaining a sampling rate of 0.00253 m^3/h. Color development of the passive sampler corresponding to chlorine exposure concentration and time was also investigated. Finally, a panel study was conducted with the help of ten volunteers who were asked to clean their bathrooms with household chlorinated disinfectants. Each panel wore the PPAS during their cleaning work, and the personal exposure level was effectively estimated after the extraction of *o*-dianisidine in the PPAS. Thus, we confirmed that the PPAS can be useful for detecting personal exposure to chlorine-based gases during indoor sanitation including COVID-19 disinfection.

Poster Presentation : **ANAL.P-238**
Analytical Chemistry
Event Hall THU 11:00~13:00

Novel Polyepinephrine-Coated $NaYF_4$:Yb^{3+}/Tm^{3+} Upconversion Nanoparticles for Selective Optosensing of Iron(III) Ions in Hela Cells and Human Serum.

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In this study, novel polyepinephrine-coated $NaYF_4$:Yb,Tm upconversion nanoparticles (UCNP@PEP) were developed through in-situ self-polymerization of epinephrine in the presence of UCNPs. The developed UCNP@PEP showed a strong blue emission (λmax = 474 nm) upon excitation with near-infrared (λex = 980 nm) light. The successful coating of UCNPs with polyepinephrine was confirmed by Fourier transform infrared spectroscopy (FT-IR). Moreover, the UCNP@PEP probes were characterized via UV-visible (UV-Vis) absorption spectroscopy, photoluminescence spectroscopy, field emission scanning electron microscopy (FE-SEM), and X-ray photoelectron spectroscopy (XPS). The developed probe has been successfully applied to detect Fe^{3+} ions with a detection limit of 0.2 μM and a good linear range of 1–10 μM. The sensing mechanism was attributed to the complexation reaction between probe and Fe^{3+} ions, thus decreasing upconversion luminescence intensity. The UCNP@PEP were tested for sensing Fe^{3+} ions in-vitro, which showed low toxicity with 90% cell viability and good selectivity for intracellular imaging of Fe^{3+} ions. Moreover, the sensor was tested for analysis of human serum and showed excellent analytical performance, thus making them an ideal candidate for sensing Fe^{3+} ions.

Poster Presentation : **ANAL.P-239**

Analytical Chemistry

Event Hall THU 11:00~13:00

Two-Photon Fluorescent Probe for Ratiometric Imaging of Cell-Membrane-Localizing γ-Glutamyl Transpeptidase

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γ-Glutamyltransferase (GGT) is a peptidase which involves in maintaining the intracellular glutathione levels and it is associated with several diseases like cancer, myocardial dysfunction etc. For reliable analysis and deep tissue imaging of biological samples it is necessary to develop a ratiometric two-photon GGT probe. In this context we have developed a benzocoumarin based two-photon ratiometric probe that can discriminate the cancer cells over the normal cells. Also this probe is featured with unperturbed signal toward pH, viscosity and polarity changes, offering an unbiased system for GGT analysis. However, the limitation of such probe is the lack of membrane-localizing ability. We attempted to develop another probe with membrane-localizing ability, maintaining two-photon and ratiometric imaging feature. For that purpose, a long alkyl chain attached naphthalene hemicyanine based probe was developed. It can discriminate normal and cancer cell as per GGT level. Also higher GGT activity was observed in tumor tissue in comparison to normal tissue. In healthy mice GGT activity was highest in kidney, however, in case of tumor xenograft mice GGT level was elevated also in colon, lung and liver. The membrane-bound probe will find practical utility in investigating GGT associated biological processes in cells and tissues by two-photon ratiometric imaging.

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Poster Presentation : **ANAL.P-240**

Analytical Chemistry

Event Hall THU 11:00~13:00

Component analysis of gastric tissue using autofluorescence

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Early diagnosis of gastric cancer is very important because it is linked to improved survival rates. However, the method used in diagnosing cancer consist of several steps that removing a part of the tissue to freezing, sectioning, staining, specimen preparation, and confirmation by a pathologist, there is a problem that at least several days are consumed before the result is confirmed. On the other hand, in diagnosis using autofluorescence, which is emitted from collagen, NADH, and FAD in living tissues, the results can be confirmed quickly without complicated procedures. However, autofluorescence in normal and cancer tissues is very difficult to distinguish due to the minute differences in the shape of the spectrum and the overall intensity, to solve this problem we used machine learning for classification. Gastric tissue is largely composed of serosa, muscle, submucosa, and mucosa layers, and the stage of gastric cancer progression is divided according to the depth of the tissue infiltrated by the cancer tissue. Therefore, we aimed to classify normal tissue and cancer tissue and classify the tissue layers. The specimen was prepared by placing the sliced tissue on quartz glass. The autofluorescence spectrum obtained by irradiating a 360 nm laser was used for machine learning. In order to construct a classification model, autofluorescence was made into image using a motor stage, which was matched and compared with a microscope image obtained by a pathologist. In addition, the accuracy of classification model was verified by comparing with the analysis results of the samples using microscope images. As a result, we distinguished the components of mucosa, submucosa, and muscle from autofluorescence images in normal tissues.

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Poster Presentation : **ANAL.P-241**

Analytical Chemistry

Event Hall THU 11:00~13:00

Optically Pumped and Matrix Assisted Anti-Stokes Raman Spectroscopy

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Anti-Stokes Raman spectroscopy is an excellent method to suppress optical backgrounds from Raman scatters and sur-rounding materials, even in electronic resonance conditions. The upshift of scattered light can avoid the fluorescence or phosphorescence that is usually red-shifted with respect to the excitation wavelength. However, this method’s competence is circumscribed by its low scattering efficiency, which results from an insufficient population of upper vibrational states that obey temperature-dependent Boltzmann statistics. To overcome this limitation, we propose that the mode-selective absorption of overtone or combination vibrations leads to enhanced anti-Stokes Raman scattering under simultaneous near-infrared (NIR) pumping and Raman excitation. Particularly, vibrationally resonant pumping is efficient for population transfer, and the excess energy is thermodynamically distributed over all fundamental vibrations. Furthermore, we present that NIR absorbing molecules can be employed as matrices to amplify anti-Stokes Raman signals of weak scattering targets.

Poster Presentation : **ANAL.P-242**
Analytical Chemistry
Event Hall THU 11:00~13:00

Time series evaluation of the diagnostic index Optical Redox Ratio

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Autofluorescence is a non-invasive analysis method which is used to diagnosing for in vivo and ex vivo tissues. Optical Redox Ratio (ORR) is a value obtained through the ratio of fluorescence intensity of Nicotinamide dinucleotide (NADH) and Flavin adenine dinucleotide (FAD). NADH and FAD are co-enzymes used in metabolism and respirations, which are strongly associated with pathological symptoms, so ORR is used as indicators for diagnosing lesion and cancer tissue. However, ORR has a various result of research on tissues and few reports have been reported on evaluating the variation of ORR value over time. In this study, we measured absorption and fluorescence over time by preparing a mixed solution of NADH and FAD at concentrations similar to biological conditions for evaluation of ORR indicators. The ORR value was obtained by decomposing each spectrum of NADH and FAD in the spectrum of the mixed solution. It was observed that the fluorescence spectral region of NADH decreased and FAD was uniform over time. This is due to the oxidation-reduction coupled reaction of NADH and FAD. In addition, fluorescence intensity of both NADH and FAD decreased when measuring fluorescence, which is an effect by the inner filter effect, and these effects tend to increase ORR values over time. Based on the spectroscopic study, we concluded that ORR values need to be calibrated before using them as a spectroscopic diagnostic marker.

Poster Presentation : **ANAL.P-243**
Analytical Chemistry
Event Hall THU 11:00~13:00

Analysis of Korean ancient glasses using Raman Spectroscopy

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Korean ancient glasses are significantly important historical sources. Especially, to know components of ancient glasses can help us determine the distribution network, the technical skills of our ancestor and the period when ancient glasses were produced. Generally, the instruments that are used to determine components of ancient glasses are ED-XRF(Energy dispersive X-Ray Fluorescence Spectrometer), EDS(Energy dispersive X-ray spectrometer) and so on. Those instruments are great tools to analyze components of ancient glasses. Operating ED-XRF, however, the samples must be under vacuum and using EDS, the samples must be preprocessed, which can be not only bothersome and time-consuming but cause destruction of samples. Although finding out the components of ancient glasses is significant, cultural assets should be conserved. Therefore, nondestructive analysis techniques are key factor to do research on cultural properties. In terms of nondestructive analysis, Raman Spectroscopy is a powerful tool. For these reasons, we employed Raman Spectroscopy to determine components of Korean ancient glasses and classify those. A 532 nm laser was used to analyze Korean ancient glasses. Depending on the groups of each glass, we could get different Raman spectra, which is caused by the differences of cation that was melted into glasses. We compared Raman spectra with EDS data and we could confirm that Raman spectroscopy can give us accurate information on qualitative analysis of ancient glasses. In addition, we suggested the possibility that by using Raman Spectroscopy we can determine the quantification information about PbO components in the lead glasses. Consequently, we note that based on Raman spectra we can do qualitative and quantitative analysis of the Korean ancient glasses.

Poster Presentation : **ANAL.P-244**

Analytical Chemistry

Event Hall THU 11:00~13:00

Quantification for unopened milk via multi-offset SORS probe

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Health has been a hot issue for worldwide people for last century and industries for health care has been grown dramatically. In particular, the interest in obesity has made people interested in fat content in food, even some countries, such as the United States and EU, recommend a low-fat diet. Accordingly, measuring the fat content of food is an important issue, and the development of its non-destructive and fast analysis method is inevitable. For the above reasons, we decided to analyze the fat content in food. Among many foods, the sample we chose is milk that is familiar and can be found in our everyday life. It also has an advantage in cost.Generally, using chromatography like GC or LC provides good enough quantitative information, but chromatography analysis is expensive, need much time, and limited in analysis without opening the milk pack. On the other hand, Raman spectroscopy is not only fast, portable, but also has the potential to analyze components in packaged materials without opening the packaging. That`s why we select SORS(Spatially Offset Raman Spectroscopy), a kind of Raman spectroscopy, the most suitable method for analyze unpacked milk. The SORS which can overcome Raman interference in the package to detect internal substances is a method for profiling depth information. In this study, we developed a line mapping multi-offset Raman probe system for quantitative analysis of fat that analyzes milk fat without opening the package. The line mapping multi-offset Raman probe system will provide accurate milk quantification information. In addition, our systems enable on-site analysis for suppliers, markets and consumers in dairy industry.

Poster Presentation : **ANAL.P-245**

Analytical Chemistry

Event Hall THU 11:00~13:00

Ultra-Sensitive Oxygen Indirect Sensing by Fluorescence Immunosandwich Assay

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Hypoxia is one of the hallmarks of the tumor environment and a prognostic factor in many cancers. In particular, hypoxia-inducible factor-1 alpha (HIF-1α) is a transcription factor involved in tumor growth and metastasis by regulating genes involved in the response to hypoxia. In this study, we developed a sensor that indirectly detects oxygen by quantifying intracellular HIF-1α concentration through fluorescence immunosandwich assay in a confined nanoregion (gold nanodisc). Qdot and Alexa were chosen as chemical probes for hypoxia imaging and indirect oxygen detection. The excellent performance of this immunoassay, with its high selectivity for HIF-1α and low detection limit (~zM), allows the determination of the amount of the biomarker (HIF-1α) in 3D spheroid cultured cancer cell lysates. It has also been demonstrated that the developed immunosensing approach is not significantly different from the results provided by generalized ELISA kits.

Poster Presentation : **ANAL.P-246**

Analytical Chemistry

Event Hall THU 11:00~13:00

Production of silver nanoparticles using microfluidic chip for SERS substrate

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In this report, we present a reproducible method to synthesize uniform-sized silver nanoparticles to apply in the fabrication of a highly sensitive SERS substrate. Using droplet as a micro-reactor, silver nanoparticles are synthesized in the channel of a droplet-based microfluidic device via reduction of silver nitrate ($AgNO_3$) by sodium borohydride ($NaBH_4$). The effect of different synthesis conditions on size distribution, dispersity, and localized surface plasmon resonance (LSPR) wavelength of the silver nanoparticles has been investigated by varying temperature, and concentrations of reactants in the aqueous phase. For fabrication of SERS substrate, the as-synthesized silver nanoparticles are arranged into a self-assembled monolayer (SAM) on liquid/air interface before depositing on silicon nanowires (SiNWs) array fabricated by one-step metal-assisted chemical etching (MACE). The fabricated SERS substrate was successfully applied for the detection of trace amounts of pesticide.

Poster Presentation : **ANAL.P-247**

Analytical Chemistry

Event Hall THU 11:00~13:00

Hybrid organic-inorganic perovskite and Eu^{3+}-complex for polyamines detection

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Polyamines, which include putrescine and spermidine, are the most basic (positively charged) tiny organic compounds found in nature. Polyamines have sparked a lot of attention due to the quick and dramatic variations in levels and ratios linked with many different types of cells that have been introduced into growth. Polyamine levels are elevated in practically all kinds of cancer, where they play a critical role in tumor growth. Halide perovskites have received attention in the optoelectronic area in recent years due to optical features such as strong photoluminescence quantum yield and adjustable emissions. Due to being biodegradable, user-friendly, less costly, and producing less trash into the environment of the paper, paper-based sensing devices have piqued the interest of many researchers in analytical chemistry. In this work, a colorimetric paper strip test was used to detect putrescine and spermidine using perovskite OAI_2PbI_4 (OPR) and Eu^{3+}-complex (Eucom). OPR-Eucom is expected as a new sensor material.

Poster Presentation : **ANAL.P-248**
Analytical Chemistry
Event Hall THU 11:00~13:00

Direct Imaging of MicroRNA in a Single Neuronal Cell Using Force-Based AFM

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MicroRNAs (miRNAs), a diverse class of 19-25 nucleotide non-coding single-stranded RNAs, play critical roles in controlling various cellular processes, and the expression levels of individual miRNAs can be considerably altered in pathological conditions such as cancer. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Detection of miRNAs has become an important emerging topic in biomedical fields. Therefore, accurate quantification of miRNAs from biological samples will lead us to better understanding of the role of miRNAs.Conventional methods widely used in the detection of miRNAs mainly include northern blotting, microarray, real-time RT-PCR and in-situ hybridization. However, conventional tools are not easy to detect high spatial localization and sensitive detection of miRNAs. Therefore, a new approach for miRNA detection method is atomic force microscopy (AFM). Force-based AFM has been used for the quantitative analysis of biomarkers. In this approach, the target molecules are captured on the surface on which target-binding molecules are immobilized, and the captured targets are recognized by an AFM tip-immobilized molecule that binds to the captured targets. By recording the specific rupture curves in a given area, the individual target molecules can be visualized. This method does not require labeling and modification, and promise superb sensitivity down to the single copy without amplification.Here, we present an AFM-based miRNA quantification and visualization method with no requisite of labeling for modification of miRNAs.

Poster Presentation : **ANAL.P-249**
Analytical Chemistry
Event Hall THU 11:00~13:00

A Study of Total Organic Carbon(TOC) in Reuse Demo Plant

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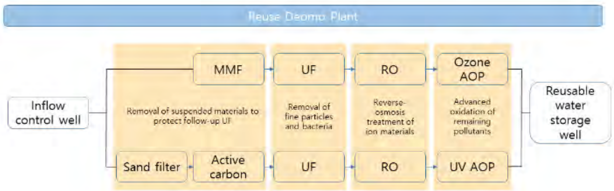
As the frequency of occurrence of water shortage in inland areas of Korea during drought is also increasing.Policies and projects to secure alternative water resources, that is, to use sewage and wastewater treatment water for industrial use, are continuously being carried out. Korea Water Cluster is developing technology for the reuse process of sewage and wastewater. Wastewater discharged from Dalseong-gun was treated and reused as raw water. The flow chart of the reuse demonstration plant is shown in the figure below. From 2022, the standard for effluent quality has changed from Chemical Oxygen Demand(COD) to Total Organic Carbon(TOC). TOC monitoring was conducted according to the flow chart of reused water.



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Poster Presentation : **ANAL.P-250**
Analytical Chemistry
Event Hall THU 11:00~13:00

Optimization of urinary small extracellular vesicle isolation using multiple cycles of centrifugation

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Small extracellular vesicles (sEV), particularly exosomes, are cell-released nanoparticles that deliver bioactive components to recipient cells, influencing the cell’s biological properties. Many studies have shown that sEV has a role in regulating physiological and pathological processes, indicating its functions as a mediator for intercellular communication. Several approaches for sEV isolation have been developed. One of the approaches is multiple cycles of centrifugation (MCC), which is similar to ultracentrifugation (the gold standard for sEV isolation) but uses a lower centrifugal speed and more centrifugation cycles. We optimized the MCC method to isolate sEV from urine by characterizing the size and related components that confirmed the presence of sEV using BCA protein assay, 1D gel electrophoresis, Western blotting, dynamic light scattering and mass spectrometry (MS). Our findings revealed that four cycles of centrifugation were sufficient to separate urine sEV, as shown by the BCA assay and ID gel analysis, where the concentration of proteins of the centrifugation cycle before the final isolated pellet was significantly reduced. The presence of sEV was confirmed by Western blotting that displayed a strong band of CD63 and TSG101 antibodies. The particle size of the final cycle was consistent between 50 and 200 nm, reflecting the typical size of sEV. A comparison of the MS spectra of supernatants and pellets showed differences in spectra profiles. After each centrifugation, MS peaks were reduced in supernatants, while the final pellet contained unique peaks associated with sEV. In this study, the MCC strategy was employed to establish the basis for future urine sEV research, particularly in the facility that lacked advanced instrumentation.

Poster Presentation : **ANAL.P-251**
Analytical Chemistry
Event Hall THU 11:00~13:00

Raman spectroscopic identification of different rice brands

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ST25 rice is a premium Vietnamese rice. The grain of ST25 rice is long with fragrance and has an appealing pineapple flavor. Moreover, since the protein content in ST25 rice is high, it becomes more attractive to people with diabetes as well as those concerning nutrition balance. Due to the high price of ST25 rice, blending with other rice varieties to gain more profits in the current market is inevitable. Therefore, to secure customer trust in purchase of goods, its authentication in market becomes more demanding and non-destructive analytical tools meeting the demand are desirable. Therefore, Raman spectroscopy able to provide rich compositional information of rice samples has been suggested. Initially, Raman spectra of ST25 and non-ST25 rice samples were acquired with sample rotation for representative spectroscopic sampling and their spectral features were comparatively analyzed. Then, the discriminability of ST25 rice samples in a principal component (PC) score domain was assessed. Meanwhile, when temperature of rice sample change, temperature-induced molecular vibrations of rice constituents is dissimilar and accordingly varied spectral feature of the sample would be more sample-to-sample characteristic. With this motivation, Raman spectra of the samples collected at different temperatures were used for analysis and subsequent discrimination results compared. Finally, two-dimensional (2D) correlation analysis effectively recognizing the temperature-induced spectral variation was adopted to potentially improve the discrimination further.**Keywords:** ST25 rice; Raman spectroscopy; Non-destructive analysis; Temperature perturbation; Two-dimensional correlation analysis

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Poster Presentation : **ANAL.P-252**
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Optimization of Solid-Phase Extraction of a Degradation Product of Novichok(A234) and its Application to Environmental Samples

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There have been no detailed investigations regarding solid-phase-extraction (SPE) optimization and screening for the degradation products of ethyl (1-(diethylamino)ethylidene)- phosphoramidofluoridate (A234) in various environmental samples. Therefore, as a first step in the selective SPE of the degradation products of A234, we optimized the SPE adsorption and extraction parameters for the A234 degradation product ethylhydrogen (1-(diethylamino)ethylidene)- phosphoramidate (cpd 1). Among various SPE cartridges, the Si cartridge (500 mg, 3 mL) selectively extracted cpd 1, using an elution volume of 4 mL of 25% H_2O in acetonitrile, which eliminated most interference without cpd 1 loss during loading and washing. In addition, the sorbent capacity is also critical in the adsorption of cpd 1. The Si cartridge (500 mg, 3 mL) retained cpd 1 in the concentration range 1–10 μg/mL. The linearity of detector response of cpd 1 in deionized H_2O was studied in range of 1.0 – 100 ng/mL, and showed good linearity with □2 ranging from 0.9979 to 0.996. The limits of detection (LODs) for cpd 1 are 10 ng/mL in the product scan mode and 100 ng/mL in the full scan mode. Also, after we optimized the SPE method, we validated precision and accuracy of the Si-cartridge extraction method in real soil samples with diverse concentrations. The precision ranged from 2.5% to 5.3%. This newly developed SPE is applicable to the analysis of a degradation product of Novichok A234 in various environmental matrices, such as water, soil, and sand, in the OPCW proficiency test and unknown samples collected from suspected sites.Keywords: chemical warfare agents, Novichok, degradation, LC-MS/MS

Poster Presentation : **ANAL.P-253**
Analytical Chemistry
Event Hall THU 11:00~13:00

MALDI-MS analysis of disaccharide isomers using graphene oxide matrix with lithium cationization agent

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Disaccharides consist of two monosaccharides joined by a glycosidic linkage. The difference in disaccharide isomers are related to their constituent monosaccharides, anomeric configuration, and type of glycosidic linkage. In this study, seven disaccharide isomers (cellobiose, melibiose, maltose, lactose, sucrose, gentiobiose, and isomaltose) were analyzed by matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) and tandem mass spectrometry (MS/MS) using a graphene oxide matrix with lithium cationization agent. The cleavage patterns of disaccharide isomers in the MALDI-MS and MS/MS analyses was different. Specific cleavage patterns were observed for each disaccharide isomer. The current results will be beneficial for differenciating disaccharide isomers using MALDI-MS.

Poster Presentation : **ANAL.P-254**

Analytical Chemistry

Event Hall THU 11:00~13:00

Comparative analysis of disaccharide isomers using GC-MS

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Disaccharide isomers such as gentiobiose, isomaltose, melibiose, lactose, maltose, cellobiose, and sucrose have the same elemental composition of C12H22O11 and the same molar mass of 342.3 g/mol. Therefore, to distinguish these disaccharide isomers additional analytical tools such as liquid chromatography (LC) or tandem mass spectrometry (MS/MS) are often required. In the case of gas chromatography (GC) - compared to LC, the compound to be analyzed for GC should be volatile. In this study, the seven disaccharide isomers were analyzed using GC-MS after trimethylsilyl derivatization. In order to compare the degree of separation of disaccharide isomers, the optimal conditions for GC separation were searched and analyzed using two different columns with different properties (DB-5MS and DB-WAX). Each disaccharide was identified as a unique GC chromatographic peak and a unique mass spectrometric pattern. The uniqueness in GC and GC-MS can be used to distinguish the disaccharide isomers. Ultimately, this study will be applicable for the qualitative and quantitative analysis of the disaccharides that are present in honey and red pepper powder.

Poster Presentation : **ANAL.P-255**

Analytical Chemistry

Event Hall THU 11:00~13:00

Pyrolysis behaviors of saturated hydrocarbons depending on their molecular weights

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The use of plastics is increasing with industrial development. Accordingly, it is reported that the amount of plastic waste increases and about 12 million tons per year of waste are released into the environment. Plastic fragments degrade and break down into small particles over time. Particles with a size of less than 5 mm are called microplastics (MPs). MPs are found in oceans, rivers, sediments, and the atmosphere. The main plastics are low density polyethylene (LDPE), high density polyethylene (HDPE), polypropylene (PP), polyethylene terephthalate (PET), polystyrene (PS), and polyvinyl chloride (PVC). Among them, LDPE and HDPE account for about 29% or more. Waxes of linear chain hydrocarbon structure in the environment are diverse. Epicuticular waxes of plants may appear together in environmental samples generated near roadside trees. In samples collected from around the road, paraffin wax contained in a tire wear particle can be detected. Recently, in the management of plastic waste, pyrolysis methods are being studied for the recycling treatment of saturated hydrocarbons such as PE and wax. Major pyrolysis products of waxes are alkanes, alkenes, and alkadiene formed by free radical reaction. We analyzed saturated hydrocarbons of different molecular weights at various pyrolysis temperatures using pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS). Pyrolysis behaviors of the saturated hydrocarbons were examined by comparing the ratios of the major pyrolysis products.

Poster Presentation : **ANAL.P-256**
Analytical Chemistry
Event Hall THU 11:00~13:00

Influence of the particle size and aging on pyrolysis behaviors of wear particles of natural rubber compound

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Road dust consists of tire wear particles (TWPs) and various wear particles caused by friction between the tire and road. TWPs have been considered as one of microplastics, and other contaminants can be attached to the surface on the road. In addition, tire wear is directly related to lifespan of tire. Therefore, a careful study is required to understand the characteristics and abrasion mechanisms of TWPs. Tires consist of rubber and various additives. In general, natural rubber (NR) is the main component of bus and truck tires. In this study, influence of the particle size and aging on pyrolysis behaviors of wear particles of natural rubber compound was investigated. Difference in the major pyrolysis products of NR wear particles according to the size and aging was examined. The wear particles were prepared using model NR vulcanizates and a laboratory abrasion tester (LAT100). The NR specimen was thermally aged in a convection oven and change of the crosslink density was also measured. The wear particles were separated using a sieve shaker by their sizes (over 1,000, 500 - 1,000, 212 - 500, 106 - 212, and 63-106 μm). Each single particle was pyrolyzed and the major pyrolysis products of isoprene and dipentene were analyzed using pyrolysis-gas chromatography (Py-GC) equipped with a furnace type pyrolyzer. Change of the abundance ratio of monomer and dimer according to the size and crosslink density was examined.

Poster Presentation : **ANAL.P-257**
Analytical Chemistry
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Ionization behaviors of dinitrotoluenes and mononitrotoluenes in atmospheric pressure chemical ionization

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Dinitrotoluenes (DNTs) and mononitrotoluenes (MNTs) are decomposed derivatives of 2,4,6-trinitrotoluene (TNT). In aerobic conditions, TNT can be decomposed to DNTs such as 2,4-dinitrotoluene (2,4-DNT) and 2,6-DNT, and the DNTs will be further decomposed into MNTs. In general, the decomposed compounds are analyzed by high performance liquid chromatography (HPLC) and gas chromatography (GC). We analyzed three DNT isomers of 2,3-DNT, 2,4-DNT and 2,6-DNT and three MNT isomers of 2-NT, 3-NT and 4-NT using atmospheric pressure chemical ionization-mass spectrometry (APCI-MS) without separation step. Detection of DNTs and MNTs can be an indicator to determine the presence of TNT. Most of DNT and MNT isomers generated [M - H]- and M.- in the negative ion mode. As the source fragmentor voltage increased, [DNT - NO]- was additionally produced. Difference in the ionization behaviors of DNT and MNT isomers was examined and the results were explained by the energy-minimized structures and energies.

Poster Presentation : **ANAL.P-258**
Analytical Chemistry
Event Hall THU 11:00~13:00

Developing catalysts for Signal amplification by reversible exchange in dimethylsulfoxide solvent system

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Nuclear Magnetic Resonance (NMR) is a powerful spectroscopy for identifying (in)organic and biological structures of molecules. The study of the dynamics of molecules is another important topic in the area of NMR studies with in biological environment. The signals in NMR depend on the population differences in magnetic field induced Zeeman splitting, which is proportional to the magnetic field, and follows the Boltzmann distribution. Hence a stronger magnetic field is better to obtain higher signal to noise. This results in high cost in preparing a strong magnet as well as maintaining the superconducting magnet. To overcome these shortcomings, hyperpolarization techniques have been developed to increase the signal intensity. Among those techniques, parahydrogen-based signal amplification by reversible exchange (SABRE) employs non-hydrogenation parahydrogen-based hyperpolarization technique with these powerful characteristics, most studies using SABRE have focused on specific solvent, MeOH due to its high efficiency. However, its polarization platform contains the deficiency in applying in the biological system. Therefore DMSO has been used as alternative since it contains not only biologically applicable but also its high solubility opens new possibilities on various hyperpolarizable substances in chemical exchange with SABRE catalyst. Here we developed new SABRE catalysts which works well in DMSO.

Poster Presentation : **ANAL.P-259**

Analytical Chemistry

Event Hall THU 11:00~13:00

Development of High Resolution 29Si MRI imaging probe based on 29Si Isotope-Enriched Silicon and Silica nanoparticles

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Dynamic nuclear polarization (DNP) technique is considered as a potential method for amplifying sensitivity of magnetic resonance (MR) imaging. Recently silicon and silica nanoparticles are in the spotlight as DNP-MRI image probes due to their biocompatibility, but 29Si MR imaging is still limited due to the insufficient hyperpolarization of nano-sized silicon nanoparticles (SiNP) and the lack of electronic defects in silica nanoparticles (SiO2 NP). To overcome the current challenges, we fabricated 29Si-enriched (10%, 15%) porous Si NPs (160 nm) and selectively 29Si-enriched core-shell SiO2 NPs by using 100% 29Si-TEOS. The physicochemical properties of particles were confirmed by SEM, TEM, and XRD. In particular, SiO2 NPs were prepared by designing a core of 40 nm and a shell of 10 nm to demonstrate the microwave penetration depth, and it was confirmed that the core-shell structure was well formed through SEM analysis. As results of DNP experiment in Si NPs, 15% enriched NPs represented ~16 times signal enhancement over natural abundance sample due to the high 29Si ratio. Furthermore, phantom imaging and animal administration were performed to demonstrate the usability of 15% 29Si-enriched particles as MRI imaging probe.In the case of core-shell SiO2 NPs, it was affirmed that the higher 29Si enrichment ratio, the improved signal enhancement, and the penetration depth of the microwave radiation was proved to about 10 nm. Currently, we are conducting research on designing particles with high signal intensity and appropriate T1 time by using TEMPOL-TEOS to select particles that can be used for MRI application.This further study is expected to increase the usability of in vivo MR imaging of SiO2 NPs by enabling self-polarization.

Poster Presentation : **ANAL.P-260**

Analytical Chemistry

Event Hall THU 11:00~13:00

Enrichment of phosphopeptides by magnetic graphene metal oxide

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Protein phosphorylation is one of the most common and vital protein post-translational modifications. Protein phosphorylation regulates proteins in numerous complex biological processes and is associated with various serious disease mechanisms. Due to the importance of phosphorylation and the low abundance, although various mass spectrometry methods have been developed to characterize phosphorylation, the enrichment of phosphorylation prior to mass spectrometry analysis is a necessary process. For this purpose, in this study, metal oxide affinity chromatography based on the affinity of the metal oxide and the phosphate group is used. Magnetic graphene with metal oxide including TiO_2, HfO_2, and ZnO have been proposed as affinity probes. The degree of complementarity of them and the complementary preference for monophosphopeptides or multiposphopeptides are compared. For the enrichment, the mixture of phosphopeptides and non-phosphopeptides is prepared by digesting beta-casein with trypsin. The magnetic graphene metal oxide (MGMO) is bound to the phosphopeptide in the loading solution (0.1 % tetrafluoroacetic acid (TFA)). And non-phosphopeptide that is not bound to metal oxides is removed through a washing stage. At this time, the MGMO can be easily separated by a magnet in order to separate the metal oxide of the phosphopeptide from the washing solution (50 % acetonitrile (ACN)/0.1 % TFA). After washing, the eluate (50 % ACN/0.1 % TFA/1 % phosphoric acid) can be added to separate the phosphopeptide and the metal oxide to obtain only the phosphopeptides. Spectra can be obtained using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry.

Poster Presentation : **ANAL.P-261**
Analytical Chemistry
Event Hall THU 11:00~13:00

Sensitive detection of SARS-CoV-2 antigen using SERS-based lateral flow assay kit with portable Raman reader

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SARS-CoV-2 has spread worldwide for over two years now. Reverse transcription-polymerase chain reaction (RT-PCR) has been considered a gold standard method for detecting the SARS-CoV-2 target gene. In RT-PCR, however, the total diagnostic time takes approximately 3-4 hours. Thus, it is necessary to shorten the detection time for rapid on-site diagnosis. Rapid antigen test kits using antigen-antibody reactions were also developed to shorten the detection time. However, they have not been adopted as a standard method due to their low sensitivity and poor accuracy. In particular, the false-negative problem of commercial rapid antigen test kits is recognized as a severe problem that can aggravate the spread of the SARS-CoV-2. To resolve this issue, we have developed a surface-enhanced Raman scattering (SERS)-based lateral flow assay (LFA) kit with a portable Raman reader for rapid and sensitive detection of SARS-CoV-2 antigen. The SERS-LFA was performed SARS-CoV-2 lysate in a viral transport medium containing nasopharyngeal swab with different concentrations of the virus (0 – 1,000 PFU/mL) and had a limit of detection (LoD) of 3.53 PFU/mL. The SERS-LFA test of SARS-CoV-2 patients was also performed for 33 clinical samples (28 positives and 5 negatives). Our SERS-based lateral flow assay kit shows a strong potential to resolve the problems in terms of low sensitivity inherent in conventional rapid kits to detect SARS-CoV-2.

Poster Presentation : **ANAL.P-262**

Analytical Chemistry

Event Hall THU 11:00~13:00

Surface-enhanced Raman scattering-based lateral flow assay strip for simultaneous diagnosis of SARS-CoV-2 and influenza A infections

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There is a high possibility that the seasonal flu is likely to spread simultaneously with severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) owing to the extended duration of the worldwide spread of COVID-19. Because SARS-CoV-2 and influenza A present similar symptoms, they are not easily distinguished without an accurate diagnosis. Therefore, when a person exhibits signs of infection, it is critical to rapidly and accurately determine which virus has infected them and initiate appropriate treatments. A colorimetric lateral flow assay (LFA) strip that can diagnose these conditions simultaneously is commercially available; however, its poor sensitivity causes a false-negative diagnosis problem. To address this, a surface-enhanced Raman scattering (SERS)-LFA strip that can simultaneously diagnose SARS-CoV-2 and influenza A with high accuracy has been developed in this study. This SERS-LFA strip provides a 100- to 1000-fold higher diagnostic sensitivity than the conventional colorimetric LFA strip. Meanwhile, it also has good clinical performance. Therefore, it is possible to identify SARS-CoV-2 and influenza A rapidly and accurately using SERS-LFA strips. Furthermore, this strip is expected to dramatically improve the false-negative diagnoses of early-stage or asymptomatic infections.

Poster Presentation : **ANAL.P-263**

Analytical Chemistry

Event Hall THU 11:00~13:00

Separation of microplastics from soil and microplastic quantification in paddy soils amended with different fertilizers

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In agricultural land, plastics such as mulching vinyl and pesticide bottles are often left unattended, and converted into microplastics through physical, chemical and biological decomposition. Although microplastics were accumulated in soil, it is difficult to quantify microplastics in soil because of lack of standard analytical methods. In soil, microplastics are separated by density differences, but organic matter in soil has low density similar to microplastics, and soil colloids are also float together, which hamper proper separation of microplastics from soil constituents. Therefore, the purpose of this study was to separate microplastics from soil and quantify microplastics in agricultural soils amended with different types of fertilizers. Microplastics comprised of polypropylene (PP), high-density polyethylene (HDPE), polystyrene (PS), and polyethylene terephthalate (PET) with different colors were spiked in farmland soil and recovery rate of the microplastics was analyzed. Alum was added during flotation of microplastics as a coagulant to remove colloids, which reduced the degree of overestimation of microplastics. Recovery rates of PP, HDPE, and PS were higher than 97%, however, recovery rate of PET was 86%. Long term amendment of compost did not significantly affect microplastic distribution in soil, but microplastics in chemical fertilizer amended soil were the higher compared to compost amended soil and no fertilized soil. PET was the most abundant in paddy soil among 4 different types of microplastics. However, PET amount in soil might be higher than measured because recovery of PET was relatively low. Therefore, the isolation method should be improved to completely separate PET from soil without extracting other soil constituents.

Poster Presentation : **ANAL.P-264**
Analytical Chemistry
Event Hall THU 11:00~13:00

SERS-based ELISA assay for Sensitive SARS-CoV-2 Detection Using Silica-encapsulated Au Core-Satellite Nanoparticles

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The enzyme-linked immunosorbent assay (ELISA) is the most widely used immunoassay technique to detect an antigen or its complementary antibody. However, sometimes it does not show sufficient sensitivity. A high-sensitivity immunoassay technique based on surface-enhanced Raman scattering (SERS)-ELISA using plasmonic nanoparticles was developed to overcome the limit of sensitivity inherent in conventional ELISA. In SERS-ELISA, SERS nanotags adsorbed to the surface of metal nanoparticles with Raman reporters were used as detection labels. When SERS nanotags are exposed to a laser beam, the incident beam intensity is dramatically enhanced by the electromagnetic enhancement effect in hot spots. Using this phenomenon, the problem of low sensitivity, inherent in conventional absorption or fluorescence ELISA, could be solved. In SERS-ELISA, however, it is critical to develop functional nanoparticles that control hot spots to realize high sensitivity and reproducibility. In this work, a silica-encapsulated core-satellite Au naoparticles (CS@SiO_2) has been developed for the sensitive detection of SARS-CoV-2. In addition, the assay was performed using a 384-well plate instead of a 96-well plate to reduce the sample amount. As a result, the low limit of detection (LOD), 8.81 PFU/mL, could be obtained, which exhibited eight times better sensitivity than a traditional ELISA. We believe that this SERS-ELISA technique has a strong potential to be a powerful tool for diagnosing various infectious diseases in the future.

Poster Presentation : **ANAL.P-265**

Analytical Chemistry

Event Hall THU 11:00~13:00

Engineered Protein Cages for Interaction-driven Selective Encapsulation of Biomolecules

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Hollow protein cages have become attractive drug delivery vehicles with high biocompatibility and precise functional/structural manipulability. However, difficulties in effective cargo loading inside the cages have been limiting further development of protein cage-based drug carriers. Here, we developed a specific interaction-driven encapsulation and cellular delivery strategy for various biomolecules by engineering a porous protein cage. The computationally designed hyperstable mi3 protein cage was circularly permuted to fuse the cancer targeting RGD tripeptide to the cage surface and SpyTag (ST), which forms a covalent bond with SpyCatcher (SC), to the cage inner cavity. SC-fused proteins with different sizes and charges could be stably and actively encapsulated in the engineered nanocage via the ST/SC reaction. Cargo protein encapsulation inside the cage was directly confirmed by Cryo-EM structure determination. In addition, SC-fused monomeric avidin was added to the nanocage to encapsulate various biotinylated (non-protein) cargos such as oligonucleotides and the anticancer drug doxorubicin. All cargo molecules loaded onto the engineered mi3 were effectively delivered to cells. This work introduces a highly versatile cargo loading/delivery strategy, where loading/delivery interactions, cargo molecules, and cell targeting moieties can be further varied for optimal cellular drug delivery.

Poster Presentation : **ANAL.P-266**
Analytical Chemistry
Event Hall THU 11:00~13:00

Classification of Soybean Paste Products Using Laser-Induced Breakdown Spectroscopy, Inductively-Coupled Plasma Optical Emission Spectroscopy, and Inductively-Coupled Plasma Mass Spectrometry

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Soybean paste is one of the most popular fermented foods consumed in East Asia. South Korea exports a large amount of soybean paste to China, and Korean soybean paste is also produced in China. In this work, the elemental analysis techniques of laser-induced breakdown spectroscopy (LIBS), inductively-coupled plasma optical emission spectroscopy (ICP-OES), and inductively-coupled plasma mass spectrometry (ICP-MS) were employed to distinguish Korean soybean pastes produced in South Korea and China from each other. 101 products from South Korea and 66 ones from China were collected to model their provenances. In the LIBS spectra, atomic or ionic emissions of Na, Cl, Mg, Ca, K, P, C, and H were identified. Among them, the emissions of Mg and C were found to possess most of the power discriminating soybean paste products from South Korea and China. From the ICP-OES analysis, the concentrations of Al, Ba, Sr, Cu, Fe, Mn, Zn, Ca, and Mg could be determined. The discrimination power obtained from these elements was found to be dominated by Mg and Sr. The provenances, South Korea and China were modeled by partial least squares-discriminant analysis (PLS-DA). The PLS-DA models based on LIBS (C and Mg) and ICP-OES (Mg and Sr) showed the discrimination accuracy of 90.3% and 91.2%, respectively. For the samples that could not be correctly distinguished, Ni, Mn, and Co, analyzed by ICP-MS, were found to provide additional independent discrimination power. The accuracy from the two-step PLS-DA model based on ICP-OES and ICP-MS reached up to 98.6%. Our results suggest that the elemental analysis techniques can provide highly reliable methodologies for screening the soybean paste products with fake origin labels.

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Poster Presentation : **ANAL.P-267**

Analytical Chemistry

Event Hall THU 11:00~13:00

A Machine Learning Approach to Identify Functional Groups from FT-IR Spectra

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Fourier-transform Infrared spectroscopy (FT-IR) is one of the most widely used analytical tools for identifying functional groups in organic/inorganic compounds. Typically, FT-IR spectral data are analyzed manually by experienced spectroscopy experts. However, these tasks are often challenging and time-consuming. Here we introduce machine learning based model for automated spectral interpretation. This model can predict the presence or absence of the 17 most common functional groups in compounds by using multi-label classification. Machine learning approaches for functional group prediction can facilitate spectral interpretation as they do not require library searches and knowledge-based analysis.

Poster Presentation : **ANAL.P-268**

Analytical Chemistry

Event Hall THU 11:00~13:00

Mesoporous Silica-Polydopamine Janus Nanoparticles for Removal Spontaneous Organic Pollutants in Oil/Water Phase

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Due to dual compositions and capabilities, mesoporous Janus nanoparticles (mJNPs) have been exploited in a variety of applications including biomedicine, catalysis, and energy storage; nevertheless, their low surface area remains a barrier. As a result, we present spherical or bowl mesoporous polydopamine (mPDA) and spherical mesoporous silica (mSiO2) Janus nanoparticles with high surface area and surface modification, which were synthesized using the Volmer-Weber heterogeneous nucleation approach. The mPDA was produced as a spherical or bowl shape using an emulsion anisotropic assembly process with a size range of 200 nm to 300 nm. The spherical mSiO2 has a diameter of 100 nm, as determined by scanning electron microscopy (SEM). The Infrared spectroscopy (FT-IR) and nitrogen adsorption-desorption (BET) were used to confirm their chemical and physical characteristics. Finally, these Janus nanoparticles were used in wastewater treatment experiments with single and dual contaminants. In order to remove spontaneous organic pollutants in the oil-water phase, we used a Pickering emulsion system of mJNPs.

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Poster Presentation : **ANAL.P-269**
Analytical Chemistry
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Investigation of DNP Spin Diffusion Barrier for TEMPOL Radical Embedded Silica Nanoparticles

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Dynamic Nuclear Polarization is a hyperpolarization technique which can be used to greatly amplify NMR signals. The hyperpolarization requires free electrons in order to create electron spins polarization which is then transferred to nuclear and enhance the nuclear spins polarization. In terms of silica nanoparticles, due to the absence of unpaired electrons, the use of exogenous species, like TEMPOL, is necessary to provide the particles with free electrons. Normally, TEMPOL is added externally into the silica powder before DNP measurement, but this leads to the limited polarization extent from particles surface (~4.2 or ~5.7 nm). In this study, we synthesized the small size TEMPOL embedded silica nanoparticles (~80nm) with homogeneous and core-shell structures for DNP measurement to investigate the nuclear spins polarization enhancement, especially, the homogeneous particles with the regular distribution of TEMPOL radicals inside can induce the polarization of the whole particles. The EPR results of synthesized silica nanoparticles confirmed the presence of TEMPOL radicals attached in the particles. In addition, the NMR measurements showed that the TEMPOL adding almost has no significant impact on the silica peaks. These results showed the promising of using these particles for further DNP experiments.

Poster Presentation : **ANAL.P-270**

Analytical Chemistry

Event Hall THU 11:00~13:00

Investigation of pH-Responsive Microcapsule based on Natural Polymers with High Applicability in Cosmetic Products

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Nowadays, functional hydrogels based on hyaluronic acid are gaining much attention because of their high applicability in cosmetics, pharmaceuticals, or foods. However, not many studies could control the shape and size of microcapsules based on this material using simple methods such as coacervation method, so we attempt to fabricate small-sized functional microcapsules with perfectly spherical shapes and investigate their intriguing stimulus-response properties. Our core-shell microcapsule is synthesized by complex coacervation method using natural polymers including sodium alginate (SA), hyaluronic acid (HA), and gelatin (GEL) as wall materials which protect active agent, vitamin E, present in core. Morphology and particle size of synthesized microcapsule were characterized by microscopy, interactions inside of microcapsule's structure were predicted through IR measurement, and UV spectroscopy also is used in encapsulated-vitamin E determination. According to microscope images, microcapsules are spherical and uniform, particle size around 20 µm to 30 µm, which is tunable by changing the HA component. Moreover, HA showed high potential in enhancing encapsulation efficiency of microcapsule, which was elucidated when EE% reached 73.8% with 1.0% w/v of HA appearance, but it only achieved 35.7% in the case of the conventional system. In addition, swelling behavior experiment performed based on the change in particle size showed microcapsules having a high swelling degree at pH 5.5, demonstrating pH-responsive characteristics of microcapsules. For further research, we will investigate more experiments to verify this microcapsule's biocompatibility and biodegradability, such as in vitro and in vivo examinations.

Poster Presentation : **ANAL.P-271**

Analytical Chemistry

Event Hall THU 11:00~13:00

Distinguishing Protein Topologies in the Gas Phase Using Supercharging Ion Mobility Spectrometry-Mass Spectrometry

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Efficient topological identification of proteins has drawn great attention in the field of protein science and engineering, because it is critical for studying topology-related biological activities of proteins and protein assemblies. However, identifying protein topologies are not trivial because the topological details are often hidden under the folded secondary and tertiary structures of proteins. In the present work, we developed a new approach combining supercharging electrospray ionization (ESI) and ion mobility spectrometry-mass spectrometry (IMS-MS) for rapid and efficient topological identification of proteins. Incorporating as many charges as possible into the proteins with supercharging, the higher-order structures of the proteins are disorganized with help of the extensive charge-charge repulsions and largely unfolded. In such cases, the topology may become significant for the geometrical size of the protein, because the impact of the secondary and tertiary folded structures on the protein conformation fades out. The maximum collision cross-section (CCS) obtained from IMS and the maximum observed charge state of the protein ion generated by supercharging ESI were proven to be excellent indices which enable us to classify the protein topologies. The chain-length-normalized maximum CCS values and charge states unambiguously divided 21 model proteins into three different groups of protein topologies: the linear, the ring-containing (lasso, circuits, and so on), and the mechanically interlocked (knots and catenanes). Furthermore, this approach has been successfully applied not only to monitor the topological transformation but also to identify any topological side product of synthetic proteins, providing a new tool for investigating protein topologies.

Poster Presentation : **ANAL.P-272**

Analytical Chemistry

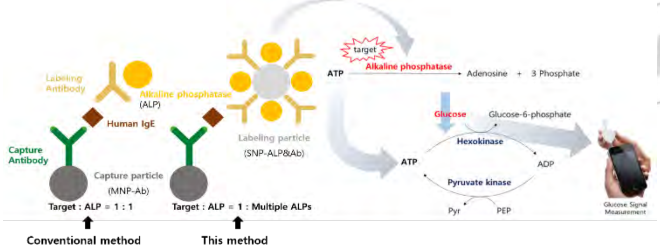
Event Hall THU 11:00~13:00

A rapid, sensitive method for detection of alkaline phosphatase utilizing a personal glucose meter.

Junhyun Park, Hyogu Han, Jun Ki Ahn*

Material & Component Convergence R&D Department, Korea Institute of Industrial Technology, Korea

These days, personal glucose meter (PGM) has been utilized for detection of non-glucose targets for point-of-care (POC) testing. We developed a new method to detect human immunoglobulin E (IgE) by glucose level with PGM. IgE is one of the major components of immediate hypersensitivity reactions that underlie atopic conditions such as seasonal allergy, asthma and anaphylaxis. Therefore, atopic disease can be diagnosed by level of human IgE in the serum. This method doesn’t require large equipment like enzyme-linked immunosorbent assay (ELISA) system as well as long reaction time. Furthermore, cascade enzyme reaction (combined with both hexokinase and pyruvate kinase) along with silica nanoparticles is exhibits highly sensitive detection performance. It is also versatile because it can detect not only IgE but also other substances if it can be linked in nanoparticles.



Poster Presentation : **ANAL.P-273**
Analytical Chemistry
Event Hall THU 11:00~13:00

Development of Micropipette-Operated Ink-Free Visual Volumetric Chip

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Visual volumetric chips based on gas-generating reactions can potentially be applied to instrument-free point-of-care testing (POCT). However, the structures of conventional chips and their detection methods are typically complicated due to two technical issues: (1) ink, as a distance marker, must be injected into a specified position before sample introduction, and (2) the gas-generating reaction must be initiated in a sealed state. In this study, an ink-free volumetric chip operated with a micropipette was developed. The volumetric chip consisted of a reaction well (R well), a substrate well (S well) containing a H_2O_2 solution as an O_2 generator, and a channel connecting the upper side of the R well and the lower side of the S well. Sample injection into the R well is followed by the insertion of a micropipette that is used to exert a negative pressure, which subsequently drives the transfer of a large portion of the H_2O_2 solution to the R well to initiate the gas-generating reaction. Meanwhile, a small portion of the H_2O_2 solution remains in the channel for use as a distance marker. The performance of the volumetric chip was evaluated by detecting Salmonella typhimurium, affording a limit of detection of 10 CFU within 20 min for culture samples and within 75 min for spiked milk samples. The volumetric chip developed herein is advantageous for POCT applications due to its simple structure and detection process.

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Poster Presentation : **ANAL.P-274**

Analytical Chemistry

Event Hall THU 11:00~13:00

Highly sensitive detection of aqueous copper(II) using multi-functional fluorescent magnetoplasmonic probes

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Department of Chemistry, Chungnam National University, Korea

Lanthanide-induced fluorescent nanomaterials are highly applicable to imaging and sensing due to their high photostability and long luminescence. These applications are based on either luminescent enhancement or quenching of fluorescent probes upon presence of analytes. In this study, multi-functional europium (Eu)-doped $Ag@Fe_3O_4$ magnetoplasmonic nanoparticles were synthesized, which emit strong red luminescence under UV excitation at 365 nm. The Eu-doped $Ag@Fe_3O_4$ fluorescent nanoparticles showed enhancement in photoluminescence intensity and quantum yield compared to the nanoparticles without plasmonic core. Furthermore, the distinctive fluorescent quenching of Eu-doped magnetoplasmonic nanoparticles (MNPs) in presence of transition metal ions were utilized to develop a sensing application. As a result of the energy transfer from Eu^{3+} fluorophore (donor) to transition metal ions (acceptor), aqueous solutions containing Cu^{2+} suffered the most from quenching effect, which were proportional to the Cu^{2+} concentration. The decrease in photoluminescence intensities showed good log-linearity in the range of 0.005-0.1 μg/mL. Furthermore, increase in sensitivity could be achieved using sample enrichment and NP separation with magnets. Therefore, Eu-doped MNPs are potential probes for sensitive detection and quantification of Cu^{2+} in aqueous samples.

Poster Presentation : **ANAL.P-275**

Analytical Chemistry

Event Hall THU 11:00~13:00

In-Vitro Toxicity Testing of Nanoparticles in Three-Dimensional Cell Culture Using MALDI Mass Spectrometry Imaging

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Three-dimensional cell culture spheroid is an effective system for fundamental research on drug penetration and nanomaterial effects that are difficult to perform in animal models. In particular, nanoparticles are essential elements in the field of nanomedicine research using functional compounds and it is very important to be toxic in vivo. We applied nanoparticles to the 3D cell culture system to investigate the effect on mammalian cells. We investigated the effect of 3D spheroid formation, growth, and apoptosis by treatment with silica (SiO_2) nanoparticle on HepG2 and HT-29 spheroids, which are liver carcinoma and colon cancer cell lines, respectively. In addition, the penetration and effect of the drug on each spherical layer, including the proliferation layer, the quiescent layer, and the necrosis layer, were investigated to confirm the possibility of expansion into nanomedicines. To this end, the imaging-based analysis that can identify cells showing changes according to the distribution of SiO_2 nanoparticles and drugs by layer in the 3D spheroids is required. We tested the toxicity of nanoparticles by introducing the matrix-assisted laser desorption ionization mass spectrometry imaging (MALDI-MSI) technique, which can acquire both local and chemical information. In this study, we established a 3D cell culture system for HepG2 and HCT-116 spheroids, and devised a method for in-vitro toxicity testing of SiO_2 nanoparticle based on MSI. In addition, in order to verify the drug effect, MALDI-MSI that can analyze the degree of permeation in the spheroid of doxorubicin, an antisense drug, and its biochemical changes was constructed.

Poster Presentation : **ANAL.P-276**
Analytical Chemistry
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Determination of Double-bond Position in Unsaturated Lipids by Ozonolysis Paper Spray Ionization Mass Spectrometry (OzPSI MS)

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Lipids are essential biomolecules as major components of cell membranes and energy sources. For lipid characterization, mass spectrometric methods have become a major workhorse, but it is hard for mass spectrometry (MS) to distinguish isomers or locate double bond(s) without employing a tandem MS (MS/MS) approach. In this study, we developed an ambient ionization platform to determine double-bond position in unsaturated lipids without performing a tandem MS experiment. The platform mainly consists of paper spray ionization (PSI), one of the simplest ambient desorption ionization methods with liquid extraction based desorption process, and an ozone-producing UV lamp. So, we called this platform ozonolysis PSI MS (OzPSI MS). Ozone produced by low pressure mercury lamp induced the cleavage at carbon double bond in lipids to form aldehyde terminals or carbonyl oxide terminals. Double bond position could be located by observing these ozonolysis products without performing tandem MS. Examples with phospholipids and long-chain fatty acids will be demonstrated in this presentation.

Poster Presentation : **ANAL.P-277**

Analytical Chemistry

Event Hall THU 11:00~13:00

Colorimetric determination of phenolic compounds using peroxidase based on hybrid nanoflowers of graphitized carbon and copper without biomolecules

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Hybrid nanoflowers consisting of graphitic carbon nitride (GCN) and copper were successfully constructed without the involvement of any biomolecule, by simply mixing them at room temperature to induce proper self-assembly to achieve a flower-like morphology. The resulting biomolecule-free GCN-copper hybrid nanoflowers (GCN-Cu NFs) exhibited an apparent peroxidase-mimicking activity, possibly owing to the synergistic effect from the coordination of GCN and copper, as well as their large surface area, which increased the number of catalytic reaction sites. The peroxidase-mimicking GCN-Cu NFs were then employed in the colorimetric determination of selected phenolic compounds hydroquinone (HQ), methylhydroquinone (MHQ), and catechol (CC). For samples without phenolic compounds, GCN-Cu NFs catalyzed the oxidation of the peroxidase substrate 3,3′,5,5′-tetramethylbenzidine (TMB) in the presence of H2O2, producing an intense blue color signal. Conversely, in the presence of phenolic compounds, the oxidation of TMB was inhibited, resulting in a significant reduction of the color signal. Using this strategy, HQ, MHQ, and CC were selectively and sensitively determined in a linear range up to 100 μM with detection limits down to 0.82, 0.27, and 0.36 μM, respectively. The practical utility of this assay system was also validated by using it to detect phenolic compounds spiked in tap water, yielding a good recovery of 97.1– 108.9% and coefficient of variation below 3.0%, demonstrating the excellent reliability and reproducibility of this strategy.Keywords Biomolecule-free hybrid nanoflowers . Graphitic carbon nitride . Colorimetric detection . Peroxidase mimics . Phenolic compounds

Poster Presentation : **ANAL.P-278**

Analytical Chemistry

Event Hall THU 11:00~13:00

Electrochemical Method for the Polymer Degradation

Jee Woo Kim, Byung-Kwon Kim*

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The molecular weight of polymers is determined by viscosity measurements, gel permeation chromatography (GPC), and nuclear magnetic resonance (NMR) spectroscopy. However, those methods generally require large amounts of polymer samples and relatively long measurement times. Therefore, a new method is required due to the difficulty of polymer analysis with the existing method. Here, we present a novel and convenient electrochemical method for analyzing the molecular weight of polymers. Using this method, the degree of decomposition of the polymer was measured. This method measures the change in the viscosity of the solvent due to the decomposition of the polymer with an electric current. This electrochemical method requires short measurement time and small amount of sample, which show great potential to analyzing and maintaining the properties of polymers in the field of industry.

Poster Presentation : **ANAL.P-279**

Analytical Chemistry

Event Hall THU 11:00~13:00

Free radical initiated peptide sequencing (FRIPS) using newly designed p-TEMPO–Bn–Sc–NHS and its application to phosphopeptide analysis

Sang Tak Lee, Han Bin Oh*

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Newly designed TEMPO-FRIPS reagent, 4-(2,2,6,6- tetramethylpiperidin-1-oxyl) methyl benzyl succinic acid N-hydroxysuccinimide or p-TEMPO–Bn–Sc–NHS, is synthesized to achieve single-step free radical-initiated peptide sequencing mass spectrometry (FRIPS MS) of targeted peptides. The p-TEMPO–Bn–Sc–NHS was conjugated to the model peptides (angiotensin II (DRVYIHPF), kinetensin (IARRHPYFL), glycoprotein IIb fragment (296-306) (TDVNGDGRHDL), and des-Pro2-bradykinin (RPPGFSPFR)) and phosphopeptides from chicken egg albumin and alpha-casein, to observe the peptide backbone dissociation patterns in MS/MS and MS3 on positive ion mode. The fragment ions that observed in single-step thermal activation of of p-TEMPO–Bn–Sc–peptides were mainly a-/x- and c-/z- type fragments and neutral loss ions, which confirms that this procedure follows the radical driven peptide backbone dissociation. Compared to the older version of TEMPO reagent, o-TEMPO–Bz–NHS, newly designed p-TEMPO–Bn–Sc–NHS has better conjugation efficiency to the targeted peptides owing to the improved structural flexibility and solubility of the reagents. The energetic interpretation using survival fraction depending on the applied normalized collision energy (NCE) ascertained the difference in the thermal activation between p-TEMPO–Bn–Sc– and o-TEMPO–Bz–C(O)– radical initiators. As the results show, the energetic effect of thermodynamic entropy by a loose transition state affects the dissociation of p-TEMPO–Bn–Sc–peptides in the FRIPS mechanism. The application of p-TEMPO–Bn–Sc– radical initiator can improve duty-cycle and the one-step collisional activation of protonated peptide precursor ions could be implemented in proteomics through the FRIPS.

Poster Presentation : **ANAL.P-280**

Analytical Chemistry

Event Hall THU 11:00~13:00

Rapid Analysis of Proteins by Droplet Paper Spray Ionization Mass Spectrometry (Drop-PSI MS) with a Hydrophobic Paper Tip

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This study investigates the use of paper spray ionization (PSI), a fast and simple ambient desorption ionization technique for mass spectrometry (MS) for rapid detection and analysis of proteins. Since a conventional cellulose-based paper substrate is too hydrophilic for proteins to be desorbed and ionized in a PSI process, various modifications on a paper substrate to increase its hydrophobicity have been suggested. Instead of modifying a paper tip in house, we tested various synthetic and natural paper that are commercially available for protein detection by PSI MS. We found that a Teslin paper, a synthetic microporous polyolefin silica matrix substrate, served as an excellent PSI tip for proteins. Since highly aqueous sample solution stays as a droplet on a Teslin PSI tip, we called this technique droplet PSI MS (Drop-PSI MS). In Drop-PSI MS, rapid protein analysis could be achieved in a ‘drop and go’ fashion and in situ modification of a sample solution was feasible. Examples of protein analysis on various PSI platforms will be demonstrated and compared. In addition, advantages and limitations of Drop-PSI MS will be highlighted and discussed in this presentation.

Poster Presentation : **ANAL.P-281**

Analytical Chemistry

Event Hall THU 11:00~13:00

In Situ Separation and Analysis of Bile Juice Using Paper Spray Ionization Mass Spectrometry

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Paper spray ionization (PSI), a simple ambient ionization method for the mass spectrometry (MS), has been employed for the rapid chemical fingerprinting analysis of the biofluid samples such as urine, blood and serum. In this study, PSI MS was employed for the analysis of the various metabolic components present in a bile juice sample, such as bile salts, phospholipids, proteins, fatty acids, and bilirubin-derived chemicals. For PSI MS analysis, one microliter of diluted bile juice was spotted onto a triangular paper tip and dried without further sample pretreatment. We tested various types of spray solvents against a bile juice sample in order to find the optimized PSI condition in terms of sensitivity and metabolite coverage. In addition to simple fingerprinting experiments, we tried to separate bile juice metabolites according to their classes during analyte transportation process in PSI. Bile salts, the most polar components in bile juice, could be clearly separated and detected from phospholipids by feeding a spray solvent into a paper tip. Our study demonstrated that PSI-MS could serve as the fast chemical fingerprinting platform for bile juice metabolites and was also able to provide wide metabolite coverage through the in-situ separation capability.

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Poster Presentation : **ANAL.P-282**
Analytical Chemistry
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Development of a quantitative analysis method of oligo-guanidines in consumer chemicals using a liquid chromatography-tandem mass spectrometer.

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Oligo-guanidine types of PHMG (polyhexamethylene guanide) and PGH (oligo (2- (2-ethoxyethyl) guanidinium), PGH (oligo (2- (2-ethoxy) ethoxyethyl) guanidinium) are disinfectants.It is often used in various commercial products such as agents, lens detergents, humidifier cleaning. However, In 2011, Humidifier disinfectant caused a large amount of life-threatening, which caused inhalation by the oligoguanidine compound in the air. It became clear that the cause was the appearance of lung disease such as lung fibrosis, which banned the use of these oligoguanidine-based substances in consumer chemicals.In this study, we developed liquid chromatography-tandem mass spectrometry (LC-MS/MS) methods for two oligo-guanidines: PHMG (polyhexamethylene guanidine), and PGH (oligo(2-(2-ethoxy)ethoxyethyl)guanidinium). The chromatography methods for each oligomer were optimized for the enhanced sensitivity together with a relatively short time run (less than 60 min). Before the quantification of oligomers, the constituents of oligomers were identified and characteristics of fragmentations were investigated by LC-MS/MS by an ion trap instrument. For the quantification of oligomers, the isotopes C13_PHMG and C13_PGH internal standard materials were selected and the calibration curve was completed. The LC-MS/MS quantitative analysis developed by triple-quadrupole showed good linearity (R^2>0.99xx) in the range of 100-1000 ppm.After that, we will extract each substance using SPE to check the recovery yield at the extraction stage and test the retention time by chromatography method.

Poster Presentation : **ANAL.P-283**

Analytical Chemistry

Event Hall THU 11:00~13:00

Towards the Laboratory Automation: From the 3D Printer Modifications

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In this study, an open-source fully automated sample preparation robot manufactured from a modification of a 3D printer was developed to be used for liquid chromatography/mass spectrometry (LC/MS) analysis. This robot was designed to perform a series of well-organized sample pretreatment steps such as micropipetting, gripping, vortexing, centrifugation, and heating block shaking without human intervention. In addition, since the auto-storage modules and transfer modules that can automatically supply the reagents required for the pretreatment process and storage the samples after the experiment have been completed, were also developed, it is able to automate whole sample preparation steps. Further, all the information needed for the fabrication, including design files, are open to the public.

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Poster Presentation : **ANAL.P-284**
Analytical Chemistry
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A Simple Colorimetric Sensor for Measuring and Recording Temperature Based on Peptide Nucleic Acid and PEGylated Graphene Oxide

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Predictive toxicology department, Korea institute of toxicology, Korea

Temperature is an important parameter in various fields, including chemistry, biology, environmentology, industry, and medical sciences. However, detection of temperature using colorimetric methods has not been sufficiently explored. In this study, we established a guanine (G)-rich DNAzyme (Dz)-based colorimetric thermosensor using peptide nucleic acid (PNA) and polyethylene glycol-functionalized graphene oxide (PEG-GO). The Dz served as a DNA template for thermosensitive nanostructures and as catalytic DNA for colorimetric assays. Using the combination of PNA and PEG-GO, we were able to control Dz activity in a thermosensitive manner, resulting in colorimetric visualization of temperature. The temperature-sensing range of this system could be simply tuned by designing a PNA strand based on the melting temperature of the Dz/PNA duplex. The programmable Dz/PNA structure with PEG-GO enabled sensitive, rapid, temperature-dependent responses. Moreover, this design permitted recall of the target temperature, enabling visualization of the temperature at a later time point. This robust system may be used as a rapid tool for practical temperature-sensing applications, such as in health diagnostics and food safety, and could be a valuable resource for basic and applied nanobiotechnology research.

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Poster Presentation : **ANAL.P-285**

Analytical Chemistry

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Simple determination of Fe3O4 concentration in sintered ores by their color images

Woosuk Sohng, Seongsoo Jeong, Hoeil Chung*

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A sintered ore consists of primarily iron oxides of magnetite (Fe3O4) and hematite (Fe2O3) with other components such as CaO, SiO2, and MgO. Since the content of Fe3O4 in sintered ore is necessary to determine for stable operation of the process, a titration method based on the redox reaction between Fe2+ and K2Cr2O7 (titrant) has been conventionally adopted; however, it is very slow and cumbersome for sample pretreatment. So, a rapid analytical method for the analysis is highly beneficial. Since the colors of Fe3O4 and Fe2O3 are black and red, respectively, the colors of sintered ores would be translated into their composition, a driving motivation for this research. With this motivation, color images (pictures) of 200 sintered ore samples with different concentrations of Fe2O3 were initially acquired. Then, 2 separate steps were employed to preprocess the image data. First, the difference in RGB values due to the change in brightness of illumination was calibrated (compensated) by using the 3D thin-plate spline warping (TPS-3D) with color-checker. Second, the shades or cracks and features of inorganic oxides except iron oxides were filtered through the image segmentation. Finally, using the 2 step-preprocessed image data, the corresponding Fe3O4 concentrations were determined using support vector regression (SVR) and resulting accuracy was comparatively discussed with that based on Raman spectroscopy. Keywords: Sintered ore; Magnetite concentration; Titration; Color image analysis; Support vector regression (SVR)

Poster Presentation : **ANAL.P-286**
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Analysis of Ni-Cr-Fe Alloys Using a Simple Low-Power Low-Resolution Laser-Induced Breakdown Spectroscopy Instrument

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Ni-Cr-Fe alloys have useful chemical and physical properties such as corrosion resistance and strength at high temperatures. Thus, they have been employed to manufacture parts used in thermal and nuclear power plants. Recently, the use of Ni-Cr-Fe is increasing particularly in the aerospace industry. In this work, the feasibility of a simple low-power low-resolution laser-induced breakdown spectroscopy (LIBS) device has been investigated for the analysis of the major alloying elements, Ni, Cr, and Fe, of the Ni-Cr-Fe alloys. LIBS is one of the elemental analysis techniques based on optical emission spectroscopy using laser-induced plasmas. It requires no or minimized sample preparation and analyzes multiple elements simultaneously and rapidly. In comparison with conventional elemental analysis techniques, the analytical performance of LIBS is inferior to theirs, but LIBS instruments can be constructed into various platforms. One of the useful LIBS platforms is a cost-effective down-sized one. A simple LIBS device was assembled using a compact low-power diode-pumped solid-state laser and a miniature spectrometer. The laser pulse energy was 270 microjoule/7-ns pulse at the wavelength of 1064 nm. This laser beam was focused on the Ni-Cr-Fe alloys (NIST SRMs) to generate plasmas. Optical emission from the plasmas was collected and dispersed by the spectrometer (spectral resolution = ~1 nm). The emission peak intensities at 547.7, 520.4, and 438.1 nm were well-calibrated to the concentrations of Ni, Cr, and Fe. Accuracy was evaluated to be 2.3, 1.2, and 3.1 wt% for Ni, Cr, and Fe, respectively, and precision was at the level of a few % in terms of relative standard deviation. Our results indicate that a simple LIBS instrument will be useful to analyze Ni-Cr-Fe alloys.

Poster Presentation : **ANAL.P-287**
Analytical Chemistry
Event Hall THU 11:00~13:00

Parahydrogen – induced hyperpolarization on metal complex : Zn(II) - tris(2-pyridylmethyl)amine)

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Metal complex is another important scaffold in body, which plays a critical role in biological environments and especially, Zn(II)-complex is one of the most abundant biological materials in body. Of successfully developed hyperpolarization techniques on Zn(II)-complex, parahydrogen-based hyperpolarization was not done on any sorts of metal complex. Here, Zn(II)-TPA is successfully hyperpolarized using SABRE, which is comparatively low-cost, fast, repeatable, portable and easy to perform for spin hyperpolarization. Comparatively small relaxation effect from Zn(II) attributes to the hyperpolarization on ligands and its polarization trend with diverse magnetic fields and Zn(II) concentrations shows distinctive from previous studies. Even though its enhancement factor is less than several pyridine derivatives, the merits of SABRE among hyperpolarization techniques would open new application in NMR-based analytical approach and hyperpolarized MRI. Most importantly, through this study, SABRE shown as great promising hyperpolarization technique but limited by relatively small polarizable substances, much wider polarizable biological materials is anticipated.

Poster Presentation : **ANAL.P-288**

Analytical Chemistry

Event Hall THU 11:00~13:00

Optimization of Headspace Gas Chromatography-Mass Spectrometry (HS-GC-MS) for Nontarget Analysis of Various Forms of Household Chemical Products

Yougyeong Park, Sangwon Cha[*]

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We are exposed to numerous household chemical products (HCPs) in our daily lives. Our health status could be significantly affected by this exposure since HCPs possess various highly volatile chemicals releasing to our living environment. Therefore, analysis of volatile chemicals, not limited to known components, from HCPs are essential for health risk assessment of HCPs. In this study, we developed a nontarget analysis (NTA) platform for volatile chemicals in HCPs with headspace gas chromatography-mass spectrometry (HS-GC-MS). Three different types of HCPs, liquid and powder detergents, and fabric softener sheet, were employed for optimization of sample preparation and HS conditions. In other words, different sample pretreatments and HS procedures like equilibration time and temperature were tested for each formula. In order to investigate the performance of the HS procedure, we compared our HS-GC-MS method with an offline solid phase extraction (SPE) followed by GC-MS. We found that our HS approach induced much less contamination during sample preparation and analysis, provided the better coverage for volatile compounds, and showed the greater reproducibility and confidence in identification than the approach with an offline extraction and GC-MS.

Poster Presentation : **ANAL.P-289**

Analytical Chemistry

Event Hall THU 11:00~13:00

Using chemoinfomatic method to predict retention time of analyzing dansylated metabolite in liquid chromatography−mass spectrometry.

Eun Woo Choi, Han Bin Oh*

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Metabolomics, the comprehensive analysis of metabolites in a biological specimen, is powerful tool to make a diagnosis and prevent several human diseases. However, metabolomics is in bottle neck. One of these bottle necks is hard to identify metabolites because of lack of information. For example, we had to know 3 kinds of information to identify metabolites in LC-MS. Retention time, accurate mass and MS/MS spectrum. We can easily find out retention time and accurate mass, however, MS/MS spectrum is not. If we can identify metabolite with these two easily finding information, bottle neck derived from lack of information can be solved. Therefore, we develop the program to deal with this bottle neck problem to identify dansylated metabolites with retention time and accurate mass. Our program consists of two parts. First part of program is predicting retention time of dansylated metabolites. Dansylation is one of the labeling techniques used at labeling metabolite containing amine or phenol. With this labeling technique, about 300 metabolites can be easily separated by LC-MS. To predict retention time, we use MORDRED to calculate descriptors, Scikit-learn to select relevant descriptors, Artificial Neural Network (ANN) to build model. Moreover, we develop program using python and our RT prediction model to predict RT of dansylated metabolite. Second part of program is fitting retention time. Retention time can be easily shifted with various reason, so we have to fit retention time. Specifically, when we know RT of some standard metabolite, we can make RT correction of these metabolites. Next, using this correction, we can predict RT of another metabolite. Therefore, we also predict RT of metabolite in different LC-MS conditions.

Poster Presentation : **ANAL.P-290**

Analytical Chemistry

Event Hall THU 11:00~13:00

Characterizing the Optical Properties of Hollow Gold Nanoshells with Plasmonic Effect

Yun a Hong, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Plasmonic gold nanoparticles are widely used as the sensor because of localized surface plasmon resonance (LSPR) effect. LSPR is the collective vibration of the surface conducting electrons when light is incident to the gold nanoparticles, along with the incident electromagnetic field. Among many gold nanoparticles, hollow gold nanoshells (HGNs) are hollow and consists of a thin gold shell and has a wider linewidth than other types of gold nanoparticles. Furthermore, HGNs have received great interest in the fabrication of biosensors due to several advantages over the solid counterparts such as high specific surface, low density, and reduction of costs. In this study, we employed dark-field (DF) spectroscopy that is a powerful tool that can visualize individual gold nanoparticles and determine their homogeneous LSPR spectra. We investigated scattering properties of single HGNs and the amplification of Raman scattering intensity by molecules chemically adsorbed on the metal surface. Therefore, we provide a deeper understanding of the characteristic optical properties of single HGNs under DF and Raman spectroscopy.

Poster Presentation : **ANAL.P-291**

Analytical Chemistry

Event Hall THU 11:00~13:00

The Effects of Chemisorption on Refractive Index Sensitivity in Mesoporous Silica Coated Gold Nanorod

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Gold nanoparticles have unique optical properties depending on their shape, size, and the refractive index of surrounding medium, caused by local surface plasmon resonance (LSPR) effect. Because of these characteristics, it is currently used in various fields such as drug delivery, photothermal therapy, biosensor, etc. In this study, we characterized mesoporous silica coated gold nanorods (AuNRs@mSiO_2), one of the gold nanoparticles with silica shell. We used dark-field (DF) microscopy and surface enhanced Raman scattering (SERS) to investigate the optical properties of single AuNRs@mSiO_2. We studied the LSPR sensitivities of two different sizes of single AuNR@mSiO_2 toward changes in the three different refractive indices (RI) of surrounding medium (air, water, oil). In addition, we used the derivative methods to improve RI sensitivity by using the inflection point. Therefore, this study provides a deeper understanding of characteristic scattering properties of AuNR@SiO_2 with different sizes as well as the effect on their RI sensitivity at the single particle level.

Poster Presentation : **ANAL.P-292**

Analytical Chemistry

Event Hall THU 11:00~13:00

Efficient Collection of Gases in Chamber System Using Impinger and the Construction of Site-specific Gas Database by GC/MS

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The chemical composition of gases collected in various environments could work as an important implication about the incident happened in specific sites. Especially, in an emergency site where the terrorism, disasters, fires, or crime occurs, the identification and relative quantitation of the gases help figuring out the cause of the incident. Due to this need, the GC/MS database for the gases generated in specific sites must be constructed. In constructing the database, gas samples in a specific site must be collected efficiently. There are several methods for the collection of gas samples on field, such as tube sampling(thermal desorption method),solid adsorption method, and using gas tedlar bag. Among the various methods, the impinger was used to collect the gas sample. In this study, a chamber was used to collect the gases in a specific space and collected gases were dissolved in an appropriate solvent for the GC/MS analysis. The MS/MS profiling and quantitative analysis of the gases were carried out to construct the database. In the future study, the same system will be applied in a field and GC/MS data of the collected gas will be used to construct site-specific gas database.

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Poster Presentation : **ANAL.P-293**

Analytical Chemistry

Event Hall THU 11:00~13:00

Comparison of quantitate analytical methods for aqueous free chlorine species

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These days, chlorine-based water disinfectants are increasingly in demand due to COVID-19. Consumer chemical products (CCPs) containing sodium dichloroisocyanurate (NaDCC) and chlorine dioxide have been widely used as an effective chlorine-based water disinfectants. The reason for their usage is chlorine's effectiveness against most of the bacteria, while its harmless characteristics to humans. However, long-term consumption and exposure to the residual chlorine in water could damage the cell membrane and even DNA. Therefore, it is important to measure the exact concentration of residual chlorine in water sample and keep the concentration below residual level. One of the difficulities in measuring the concentration of chlorine species in water comes from their highly reactive characteristics. Aqueous chlorine species exist in various chemical structures like chlorine dioxide, hypochlorite and hypochlorous acids. Therefore, it is impossible to specifically measure certain type of chlroine species. Colorimetric measurement of chlorine using (DPD), or DPD method, has been the standard method for measuring the free chlorine in water sample. NaDCC has a special property. When it's dissociated in water, it exists in two states, HOCl and cyanuric acid. It is necessary to quantify the absorption intensity of cyanuric acid by maintaining a constant pH using an appropriate butter. We will use several spectrometers to find better analytical method for aqueous free chlorine species.

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Poster Presentation : **ANAL.P-294**

Analytical Chemistry

Event Hall THU 11:00~13:00

Optimization of n-doped hydrochar derived from withered flowers

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Many studies are being conducted to convert various biomasses into valuable substances. The withered flowers were carbonized by hydrothermal carbonization (HTC) followed by activation with n-doping materials. Reaction parameters involving HTC reaction and activation were optimized using the design of experiments (DOE). The HTC conditions were temperature, time, and amount of sample while activation conditions were temperature, a mass ratio of n-doping material and KOH. Methylene blue number (MBN) was measured for each n-doped hydrochar to determine the reaction parameters. The physicochemical and electrochemical properties were measured for the n-doped hydrochar synthesized at the optimized condition. After the activation conditions are optimized, the specific capacitance will be calculated through CV, GCD, and EIS measurements.

Poster Presentation : **ANAL.P-295**

Analytical Chemistry

Event Hall THU 11:00~13:00

Symmetry Breaking of Chiral Nematic Structure film for DNA Sensing

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Symmetry breaking has been known as the origin of chirality where the asymmetric interaction between circularly polarized light and chiral nanostructure varies circular dichroism. In this experiment, we made the plasmonic nematic film(PNF) using Ag@Fe3O4 and sensing DNA with PNF. We showed symmetric breaking by placing Au NPs between MagPlas NPs layers.

Poster Presentation : **ANAL.P-296**
Analytical Chemistry
Event Hall THU 11:00~13:00

Analytical strategies for determination of glycosidic linkages of disaccharide isomers derived from polysaccharides using PGC-LC/MS

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Polysaccharides are the most abundant biomolecules in nature. They are usually made up of different bonds of several monosaccharides and are of different types depending on the linkage structure. For example, amylopectin and cellulose, which are made from the most glucose in nature, are α(1→4) glucose and β(1→4) glucose polysaccharides respectively. Although important bioactive functions of polysaccharides are known according to such a linkage structure, studies are lacking due to structural similarity of polysaccharides. The ideal polysaccharide structure analysis is to use an enzyme that cleaves the specific linkage site. However, the current analysis is performed by random cleavage through acid hydrolysis because enzymes are not available in all polysaccharides. In this study, we established an analytical strategy to distinguish disaccharide isomers based on PGC-LC/MS to analyze the linkage of polysaccharides. 1) Disaccharides were constructed through mild acid hydrolysis of polysaccharides. 2) A reduction method is performed to reduce separation by extra isomers in the chromatogram, and only disaccharides are enriched using a PGC-based solid phase extraction method. 3) PGC-LC/MS was used to separate the disaccharide standard, and the disaccharide obtained from the polysaccharide was identified by matching the retention time and mass value. Our strategy was demonstrated by applying to a polysaccharide standard having a glucose α(1→6) linkage structure. This analytical strategy can quickly identify the linkage structures of polysaccharides and serve as one of the general platforms for future polysaccharide structure analysis.

Poster Presentation : **ANAL.P-297**

Analytical Chemistry

Event Hall THU 11:00~13:00

The efficacy of prostate cancer diagnosis using PSA between blood test and cancer tissues

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As a protein biomarker, prostate-specific antigen (PSA) in blood has been widely used for the early diagnosis of prostate cancer (PCa) in clinics. However, PSA also increases in other prostate diseases, such as benign prostatic hyperplasia (BPH) and prostatitis. This leads to a higher number of false positives and causes unnecessary biopsies, an invasive procedure which is associated with risks including bleeding and sepsis. This study intended to identify PSA information from different prostate cancer tissues with different PSA values in patients' blood to discover relationship between blood and cancer tissues for a more accurate early diagnosis.PCa tissues were collected from the PCa patients, homogenized, and proteins were extracted from the homogenized PCa tissues. Then each supernatant fluid was trypsin digested and desalted respectively, and the proteins in all PCa tissues were identified and quantified using nLC-MS/MS and protein database search softwares.

Poster Presentation : **ANAL.P-298**

Analytical Chemistry

Event Hall THU 11:00~13:00

Magneto-Plasmonic Metasurface sensor at Terahertz regime for biosensing

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Terahertz (THz) waves have great potential for wide applications in imaging, sensing, and other fields. However, due to the lack of strong response materials for efficient generation, and detection of THz waves, many researchers introduce metamaterials that afford the generation, polarization, sensing, and imaging THz waves. Metamaterials, artificially designed electromagnetic materials arranged with subwavelength structures, can be designed by changing their unit cell. Herein, new THz metamaterials, Ag@Fe3O4 magneto-plasmonic (MagPlas) nanoparticles (NPs) are coated on the unit cell of the nickel-patterned metasurface. By magnetizing metasurface, NPs can be assembled with the ferromagnetic properties of nickel on the surface. On the magnetized metasurface with MagPlas NPs, THz resonance with improved sensitivity of hearing loss DNA sensing. That biomarker, hearing loss DNA, in pregnant woman who are at high-risk of pregnancy with single-gene disorders have been presented in 400 genetic syndromes. A combination of metamaterials and MagPlas NPs was exploited to develop an ultrasensitive THz biosensor with high sensitivity. Using this platform, hearing loss DNA can be combined with NPs, which shows the potential for development to the biosensor.

Poster Presentation : **ANAL.P-299**

Analytical Chemistry

Event Hall THU 11:00~13:00

Superlocalization of Intracellular Organelles in Live Single Cells by Three-Dimensional Light Sheet-based Superresolution Microscopy and Cubic Spline Algorithm

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The contact distance between the mitochondria (Mito) and the endoplasmic reticulum (ER) has received considerable attention because of its important function in maintaining lipid and calcium homeostasis. In this study, the Mito-ER contact distance in living single cells was observed using a three-dimensional light sheet-based superresolution microscopy (3D LSRM) and a cubic spline algorithm. To maintain photobleaching and photostability, the Mito and ER were conjugated with plasmon nanoparticles (12 nm gold nanoparticle and 20 nm silver nanoparticle). In the 3D superresolution images of Mito and ER, the average distance between Mito and ER was 22.4 nm in HeLa cell, 22.2 nm in RAW264.7 macrophage, 21.4 nm in AGS cell and HT29 cell, and 21.3 nm in HEK293 cell, respectively. This result showed 88% similarity to the results obtained by electron microscopy in both normal cells and cancer cells. The 3D LSRM with cubic spline algorithm improved the centroid positioning accuracy for nanoparticle conjugated intracellular organelles, contributing to the spatiotemporal measurements between objects. Moreover, this method can be applied to study the intracellular structure of various live single cells at subdiffraction limit resolution.

Poster Presentation : **ANAL.P-300**

Analytical Chemistry

Event Hall THU 11:00~13:00

Single-Particle Spectroelectrochemistry: Electrochemical Tuning of Plasmonic Properties via Mercury Amalgamation in Mesoporous Silica Coated Gold Nanorods without Structural Deformation

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This paper presents the elucidation of the mercury (Hg) amalgamation induced by electrochemical reduction on gold nanorods coated with mesoporous silica shell (AuNRs@mSiO_2) by single-particle spectroelectrochemistry. First, the silica shell significantly enhanced the structural stability of AuNR cores after Hg amalgamation with application of linear sweep voltages (LSVs). Thus, it became possible to focus on the spectral changes of AuNRs@mSiO_2 induced by the deposition of Hg without disturbance of structural deformation that also strongly affects the localized surface plasmon resonance (LSPR) properties. Second, following the application of LSV in the presence of Hg^{2+}, a remarkable blue shift of LSPR peak was observed, caused by lowering of the work function due to the Hg adsorption, donating electron density to Au. Furthermore, the LSPR linewidth also showed a dramatic increase after the Hg deposition with LSV. Last, direct observation of the evolution of the Hg amalgamation process was presented by monitoring real-time LSPR peak and LSPR linewidth shifts of single AuNRs@mSiO_2 in the Hg solution according to application of electrochemical potential. Moreover, the results showed the possibility of in-situ tuning of the LSPR properties of AuNRs@mSiO_2 by the Hg deposition via electrochemical potential manipulations without disturbance of structural variations of AuNR cores.Keywords: Spectroelectrochemistry, Au-Hg amalgamation, Gold nanorods, Mesoporous silica shell, Single particle spectroscopy, Localized surface plasmon resonance

Poster Presentation : **ANAL.P-301**

Analytical Chemistry

Event Hall THU 11:00~13:00

Two-dimensional iron selenide nanoarchitecture synthesized by solvothermal, and their characterization

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Two-dimensional (2D) layered structures, such as graphene, black phosphorus, TMD, and Mxenes, have attracted substantial attention in recent years as a group of potentially high-performance thermoelectric materials. In particular, layered iron chalcogenides provide excellent properties to study intertwined phase transitions, superconductivity, and magnetism, as promising platforms for the conversion of renewable solar energy to chemical fuel to their unique optoelectronic, transport, and interfacial properties. Herein, we report a design strategy for 2D FeSe lateral nanoplate to achieve considerable promise for energy conversion and optical devices. The atomic structure of FeSe is confirmed by X-ray diffraction and transmission electron microscopy. Moreover, the series of mechanistic studies clearly demonstrate the growth strategy of the 2D FeSe thermoelectric materials as well as the background for growth into the two-dimensional structure. Layered iron chalcogenides will be potential candidates to explore novel quantum physics and other applications.

Poster Presentation : **ANAL.P-302**

Analytical Chemistry

Event Hall THU 11:00~13:00

Structural studies of human Amyloid protein forming ion channel using NMR spectroscopy

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Amyloid beta (Aβ), known to play a major role in the pathogenesis of Alzheimer’s disease, is a fragment separated from amyloid precursor protein (APP). APP is a transmembrane protein that penetrates the neuron’s membrane. The hypothesis for ion channel formation of Aβ is that the ion channels in the nerve cell membrane induced by accumulated Aβ disturbs calcium ion homeostasis and causes Alzheimer’s disease. Due to the formation of these ion channels, the concentration of ions inside the cell is changed, which can cause neuronal cell death and memory impairment. Many studies have been conducted on substances that block or inhibit the formation of such ion channels, and one of them is zinc ion. Zinc ions bind with strong affinity to the Aβ ion channels, blocking one side of the ion channels and reducing their conductivity which is implied a decrease in the flow of calcium ions, the possibility of restoring calcium ion homeostasis in nerve cells. This study focused on APP containing an amino acid sequence including residues 692-723 of the transmembrane region (hAPP-TM) which is known that it has an affinity for zinc ions. We demonstrated the effect of zinc ions to close the ion channel of Aβ protein via structural changes using solution/solid-state NMR in membrane proteins.

Poster Presentation : **ANAL.P-303**

Analytical Chemistry

Event Hall THU 11:00~13:00

NMR Structural Analysis of the Syndecan-4 receptor with transmembrane domain

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The syndecan family is heparan sulfate proteoglycans, which consist of a core protein and heparan sulfate. Of the syndecan family, syndecan-4 is a very important factor in relation to cancer through interaction with growth factor receptor (GFR). It performs functions such as growth factor receptor activation and cell-cell interactions and is implicated in tumor suppression.Syndecan-4 has an extracellular domain composed of (ecto-), transmembrane (TM), and cytoplasmic (Cyto-) domains, and an intracellular domain composed of C1, V (variable region), and C2 domains. Syndecan-4 is a transmembrane protein that transmits stimuli to cells via PIP2 (phosphatidylinositol-(4, 5)-bisphosphate) phospholipids. The 183th residue of syndecan-4, serine, is dephosphorylated to activate PIP2 and activate protein kinase Cα. Besides, activation of protein kinase Cα activates cytoplasmic calcium and hormone binding involved in promoting tumor growth. The part that directly binds to PIP2 is the V region, and the signaling process occurs through the cell surface receptor protein in the transmembrane domain. Syndecan-4 forms dimer by the GXXXG sequence in the cell membrane region. Although the dimerization reaction of syndecan-4 cell membrane appears to play an important role in its function, few studies have been conducted on the cell membrane region.An experiment was conducted to see what structure it had in the membrane of Syndecan-4. Syndecan4-eTC (ecto-, TM, Cyto-) domain-containing Syndecan-4 expression and purification process was optimized. In addition, we experimented with solution/solid NMR spectroscopy to confirm the structure and interaction.

Poster Presentation : **ANAL.P-304**

Analytical Chemistry

Event Hall THU 11:00~13:00

Metabolomic analysis in liver tissues from mouse model to determine the role of AMPK activator in NASH using LC-MS

Yeajin Ju, Jueun Lee*, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Non-alcoholic steatohepatitis (NASH) is a risk factor for hepatocellular carcinoma lead to liver cell damage and inflammation along with fatty deposition. AMP-activated protein kinase (AMPK) plays an important function in controlling energy homeostasis and the activation can inhibit NASH pathology. However, the effect of the AMPK activation on hepatic metabolic rewiring remains unknown.This study aimed to investigate the therapeutic effects of AMPK on hepatic metabolism on NASH using metabolic analysis. C57BL/6J male mice were fed a choline-deficient high fat diet (CD-HFD) for 6 weeks to induce NASH and treated them with YE-21, a new direct AMPK activator candidate, every 2 days for 14 times. Then, we performed metabolic profiling of liver tissue using ultra-performance liquid chromatography–quadrupole time-of-flight mass spectrometry. Mice were divided into four groups: control (n=12), YE-21 (n=12), CD-HFD (n=12), and CD-HFD+YE-21 (n=12). We observed strong separation among three groups of control, CD-HFD and CD-HFD+YE-21 mice in partial least squares-discriminant analysis score plots. A total of 92 metabolites were identified in positive and negative mode. To find key metabolic pathways after YE-21 treatment in mice fed CD-HFD, pathway analysis was performed using significantly different 17 metabolites between CD-HFD and CD-HFD+YE-21. As a result, the most enriched metabolic pathways were cysteine and methionine metabolism, pyrimidine metabolism and amino sugar and nucleotide sugar metabolism. In particular, s-adenosyl homocysteine significantly increased in CD-HFD+YE-21 compared to CD-HFD, whereas cystathione and glutathione oxidized (GSSG) were significantly decreased in CD-HFD+YE-21 compared to CD-HFD in cysteine and methionine metabolism. Our finding suggested that YE-21 might improve liver damage and fibrosis due to NASH by regulating hepatic metabolism, and demonstrated that metabolic profiling is a useful method to investigate the therapeutic effects of AMPK activation in diet-induced NASH mice.

Poster Presentation : **ANAL.P-305**

Analytical Chemistry

Event Hall THU 11:00~13:00

Crosslink of metabolic alternations between liver and adipose tissues in mouse models with nonalcoholic steatohepatitis (NASH)

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Nonalcoholic fatty liver disease (NAFLD) is recently recognized as one of the most prevalent etiologies of chronic liver disease, affecting 25% adult population worldwide. NAFLD represents a wide spectrum of diseases ranging from nonalcoholic fatty liver (NAFL) and the progressive form as nonalcoholic steatohepatitis (NASH). However, there is a lack of investigation summarizing organ metabolic changes in NASH model. In this study, we examined the metabolic changes in liver and adipose tissues of mice (n=47) using liquid chromatography/triple quadrupole mass spectrometry (LC/TQ-MS) for polar extracts. Control group was fed with chow diet for 3 weeks whereas NASH groups were fed with high fat diet (HFD) for 3,10,33 and 43 weeks, and mice were sacrificed at each time point. Total 8 classes of polar metabolites were found from semi-targeted polar analysis and then Mann-Whitney test was performed to compare alternations between group and ahead group along NASH progression in liver and adipose tissues. For polar metabolites, amino acids represented similar trend along the period of NASH diet fed in liver and adipose tissues. Intriguingly, change of branched chain amino acids and aromatic amino acids first appeared in liver tissues compared with in adipose tissues. This study demonstrates LC-MS/MS based metabolic profiling is a useful tool to detect characteristic changes along HFD feeding period in liver and adipose tissues.

Poster Presentation : **ANAL.P-306**

Analytical Chemistry

Event Hall THU 11:00~13:00

Expression and NMR structural studies of antimicrobial peptides, Lactophoricin

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Antimicrobial peptides (AMPs) are highly notable cause of its biochemical properties. Although many native AMPs have been discovered and researched so far, they have rarely used as therapeutic agent because of their problems such as in vivo stability issues. But, unlike antibiotics, AMPs are not influence for appearance of many multidrug-resistance bacteria or super bacteria result from abuse of antibiotics. By this reason, AMPs still have potential for producing good pharmaceutical drugs. The AMPs studied in this research are analogs of Lactophoricin-YK5 (LPcin-YK5). Lactophoricin- I (LPcin- I), origins of LPcin-YK5, is a cationic amphipathic peptide consists of 23-mer peptide from bovine milk. Through peptide engineering based on LPcin-I, we designed and purified LPcin-YK3 peptide. LPcin-YK3 is a novel AMP with shorter length, higher activity and less toxicity than lactophoricin. After that, we developed YK5 peptide by using the YK3 peptide. In this process, we increased positive charge value of peptide so that the entire peptide can bind with negatively charged bacterial cell wall more easily. Also, the polar residue was replaced with a nonpolar surface to give imperfect amphipathic properties. Based on the methods mentioned above, we designed YK5 which has higher antimicrobial activity.LPcin analog peptide was produced and obtained with high yield and purity by using a gene recombinant method. Then we analyzed structural properties of analog peptide by spectroscopic methods such as MALDI-TOF, CD.

Poster Presentation : **ANAL.P-307**

Analytical Chemistry

Event Hall THU 11:00~13:00

Expression and Purification of human melanocortin-4 receptor for NMR structural study

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Human transmembrane proteins (hTMP) are a component of biological membranes and play a very important role in biological systems such as signal transduction receptor function, cytoskeleton, and signal transduction. Therefore, when the membrane proteins are mutated, it can be linked to various diseases. It can also lead to loss of function as a carrier of substances and disruption of signal transmission systems. To understand the function of membrane proteins, it is essential to know the three-dimensional structure and information.Among them, it deals with the human melanocortin-4 receptor (hMC4R), which is expressed in the pituitary gland and functions to maintain energy homeostasis. Mutations in the melanocortin-4 receptor, which are closely related to appetite regulation, cause genetic obesity in human. This study mainly deals with the process of optimizing the expression, isolation, and purification process, which is the process of obtaining a high-yield wt/m-hMC4R-TM2 protein for high-quality NMR structural studies. It has been applied to various spectroscopy methods including solution-state NMR spectroscopy and solid-state NMR spectroscopy to investigate the structural differences of expressed wt/m-hMC4R-TM2.

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Poster Presentation : **ANAL.P-308**
Analytical Chemistry
Event Hall THU 11:00~13:00

Metabolomic analysis of brain tissues from mice exposed to ambient particulate matter using LC-MS approach

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Ambient particulate matter(PM) has become major environmental risk factors to public health, and related to human diseases including respiratory disease, cardiovascular and nervous disorder. However, the effect of exposure to PM has not been fully understood in a biological system. We observe the metabolic changes in response to PM with a diameter 2.5-10 μm (PM10) exposure in mouse model.In this study, C57BI/6J mice (male) were exposed to PM10 or clean air for 3 weeks in chambers. We conducted a targeted analysis of cortex and cerebellum from mice to assess the metabolic perturbations using ultra performance liquid chromatography/triple-quadrupole mass spectrometry (UPLC/TQ-MS). Partial least squares - discriminant analysis (PLS-DA) score plots showed a clear separation between the PM10 exposed group and the control group. We observed the changes in endogenous metabolites related to neurotransmitter and amino acids including alanine, aspartate and glutamate metabolism and valine, leucine and isoleucine biosynthesis in PM10 exposed mice compared to control. Branched-chain amino acids (BCAA) were significantly upregulated in PM10 exposed group, indicating the alteration in BCAA metabolism.This study demonstrates that the LC-MS based-metabolic profiling can be used to understand the metabolism of PM10 exposed group on biological systems.

Poster Presentation : **ANAL.P-309**

Analytical Chemistry

Event Hall THU 11:00~13:00

Ostwald Ripening of FeSe nanoparticles in Organic Solvents

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Ultrathin transition metal chalcogenide nanosheets were suggested for many categories of applications, such as electrocatalysts for oxygen evolution reactions(OER), biosensors, or electrodes for supercapacitors. In this research, the experimental purpose is making ultrathin FeSe nanosheets which is one of the transition metal chalcogenide material, synthesized in organic solvents, and exfoliating them to make monolayered FeSe nanosheets. A lot of methods were already suggested to exfoliate multilayered transition metal-based materials into one layer. However, even though some of the strategies were effective to produce monolayered nanosheets, they still have disadvantages, like spending too much time, redeposition on the produced monolayered nanosheets surface. Therefore, the ostwald ripening driven exfoliation(ORDE) strategy has been applied to our exfoliation experiment to make effective result. Herein, the trials to make monolayered FeSe nanosheets from three-dimensional FeSe nanoparticles, and TEM images, optically analyesed results of the products were described.

Poster Presentation : **ANAL.P-310**
Analytical Chemistry
Event Hall THU 11:00~13:00

Optimized expression and NMR structural studies of Anti-inflammatory tIK peptid

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Rheumatoid arthritis is an autoimmune disease caused by an imbalance between pro-inflammatory and anti-inflammatory cytokines. Inflammation in the joints damages ligaments and cartilage, spreads throughout the body through blood vessels, causing fatigue and anemia, and in severe cases leads to dangerous complications. Recently, it has been revealed that a specific amino acid sequence of the truncated-IK (tIK) protein suppresses the expression of inflammatory cytokines. Therefore, we conducted research to develop therapeutic candidates by finding the portion expressing anti-inflammatory properties in the peptide. We tested phosphorylation patterns in macrophages from tIK transgenic mice and found that the tIK protein phosphorylates tyrosine 496th of the interleukin (IL)-10 receptor subunit alpha. As a result of predicting a specific fragment of tIK protein that induces phosphorylation by comparing the structure of IL-10 using sequence homology modeling, four epitope candidate groups were found. In order to confirm the anti-inflammatory activity of each epitope, candidate groups were compared through a T_H17 cell differentiation test, and it was confirmed that the epitope consisting of 18 amino acids had the best anti-inflammatory properties. Derived from this peptide, two with shorter amino acid sequences were also found.The peptide was expressed by culturing *E. coli* in which the N of the amino group in the peptide was substituted with ^{15}N. It was analyzed by MALDI-TOF and NMR. CD and 2D NMR experiments were conducted to study secondary structure of the peptides, and the interaction with the receptor was studied using chemical shift perturbation.

Poster Presentation : **ANAL.P-311**

Analytical Chemistry

Event Hall THU 11:00~13:00

Scale-up synthesis of high fluorescent FeSe quantum dot in aqueous condition

Yujin Choi, Jaebeom Lee*

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Iron chalcogenides hold considerable promise for energy conversion and biomedical applications. These iron-containing quantum dots also serve as a safe alternative to the conventionally used metal-chalcogenide systems in which the heavy metal component is usually toxic. Here, a successful synthesis of Iron selenide(FeSe) quantum dots(QDs) is reported in an aqueous system using glutathione(GSH) and L-cysteine(Cys) as surfactants. The reaction was optimized by controlling reaction pH, time, and temperature to improve the quantum yield. Then, the QDs with the highest QY were characterized by transmission electron microscopy (TEM) and optical spectrophotometry. Scale-up synthesis was carried out where 100~1000mL reactors were used to synthesize QD up to 0.1g per batch. Furthermore, the prepared FeSe NPs exhibited intense light blue fluorescence on ultraviolet light exposure, which also displays strong photoluminescence and relatively high quantum yield in an aqueous system(c.a.20%). This novel strategy, based on the synthesis of Iron chalcogenides quantum dots in an aqueous system, has the potential to increase significantly towards in-vivo bio-imaging and sensing.

Poster Presentation : **ANAL.P-312**

Analytical Chemistry

Event Hall THU 11:00~13:00

Synthesis and characterization of fluorescent-doped iron oxide nanoparticles

Hwayoung Choi, Jaebeom Lee[1,*]

Department of Chemistry, Chungnam National University, Korea
[1]*Chemistry, Chungnam National University, Korea*

Lanthanide-doped nanomaterials exhibit unique optical properties, such as large Stokes shift, sharp emission peaks with narrow bandwidth, low photobleaching, stability to photochemical degradation, low toxicity, and the absence of blinking. Therefore, it has been widely used for various biomedical applications. Among them, europium-based nanomaterials are better candidate for bioimaging, therapeutics, immunoassay due to the long luminescent lifetime and low background signals. In this study, lanthanide-doped magnetic nanoparticles were synthesized, which have magnetic and fluorescent properties and were characterized by UV-Vis absorption, photoluminescence (PL), and scanning electron microscope (SEM).

Poster Presentation : **ANAL.P-313**

Analytical Chemistry

Event Hall THU 11:00~13:00

Synthesis of FeSe quantum dots in the organic phase and ligand exchange

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Quantum dots(QDs) are one of the outstanding discoveries in nanoscience, for example, when their electrons are excited by receiving energy, QDs emit diverse colors depending on their sizes. These QDs have been successfully applied in various fields such as optics, electronics, and biology. Existing quantum dots use rare heavy metals and are expensive therefore they have limited applications. Herein, we report the one-pot synthesis of FeSe QDs in the organic phase for high quantum yield and ligand exchange method from organic phase to aqueous phase. The high crystallinity of the QDs was confirmed by transmission electron microscopy (TEM) with an average size of 3.5 nm. Although the quantum yield of the aqueous phase is lower than that of the organic phase, the quantum yield is more than 20%.

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Poster Presentation : **ANAL.P-314**
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Plasmon-Induced Photopolymerization of Acrylic acid in Au colloids under a Monochromatic Laser Illumination

Jeonghyeon Lee, Youngsoo Kim*

Department of Chemistry, Yeungnam University, Korea

Polymer/nanoparticle hybrid nanocomposites have been receiving much attention as a potential material in a broad range of applications like catalysis, drug delivery, sensing, therapeutic materials, and electronic materials. Although diverse synthesis strategies for obtaining polymer/nanoparticle composites have been proposed, photopolymerization is one of the most powerful tools among other methods proposed. In general, it is well known that the photopolymerization at the vicinity of nanoparticles took place by either electron transfer or photothermal effect using a pulse laser system. However, the mechanism of photopolymerization on the surface of nanoparticles by the electron transfer and photothermal effect is still being competitive. In this work, we conducted photopolymerization to reveal the polymerization mechanism of polymer/nanoparticle nanocomposite in the Au colloid system under the continuous-wave laser illumination with different excitation wavelengths, and the polymerization of acrylic acid (AA), which is the simplest system, was chosen as a model system. We investigated the main influence of photo-induced polymerization by controlling incident wavelength, polymerization time, reaction conditions, and etc. By using a UV-Vis spectrophotometer, we monitored the Au LSPR shift of the synthesized PAA@Au NPs to observe the change in dielectric constant around the Au NPs and the morphological change was confirmed using TEM. Also, we identified the chemical state of the products using other analytical tools like Raman spectroscopy and MALDI-TOF.

Poster Presentation : **ANAL.P-315**

Analytical Chemistry

Event Hall THU 11:00~13:00

Preparation of Steady-Staying Gold Nanoparticles at Aqueous-Organic Phase Interfaces

Juhee Ha, Youngsoo Kim*

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Gold nanoparticles (Au NPs) have been receiving great attention as potential photocatalysts owing to superior catalytic properties at the nanoscale regime and unique optical properties resulting from the localized surface plasmon resonance (LSPR) when they interact with visible light. Therefore, gold nanoparticles have been used as a photocatalyst to drive important photochemical reactions like CO_2 reduction, H_2 dissociation, and epoxidation. Recently, many studies have been reported the diverse cases of organic synthesis, which was achieved green chemistry, using nanoparticle-based photocatalysts driven under the visible light. Because the nanoparticles are dispersed in only a single phase of liquid, however, the scalability of organic synthesizes using nanoparticle-based photocatalysts is critically limited. To overcome these issues, and apply to diverse organic reaction models, it is important that Au NPs, which are photocatalysts, should be having a dual degree of dispersion in aqueous-organic phase, simultaneously. In this study, we demonstrated synthesizing gold nanoparticles capped with dual phase ligand through the surface engineering that controlled the type and ratio of ligand. The Au NPs were characterized by transmission electron microscope (TEM), atomic force microscopy (AFM), electrophoresis, and dynamic light scattering (DLS). We hope that the staying gold nanoparticles at aqueous-organic interfaces can expand the availability of nanoparticle-based photocatalysts in organic synthesis.

Poster Presentation : **ANAL.P-316**

Analytical Chemistry

Event Hall THU 11:00~13:00

Structural and electrochemical studies of fluorine substituted $LiFe_{1-x}Mn_xBO_3$ as a cathode material for Li–ion battery

Daeun Han, Jimin Kim, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

Among the cathode materials of lithium-ion batteries, borate-based materials have been studied by many researchers due to their high theoretical capacity (220 mAh g^{-1}). $LiFeBO_3$ has good reversible capacity and safety with low open-circuit voltage (OCV). In previous studies, we have shown the improved discharge capacity by fluorine substitution in oxygen site of $LiFeBO_3$ but having structural instability. In this study, to increase structural stability, manganese has been applied to the iron site in F substituted $LiFeBO_3$ and $LiFe_{1-x}Mn_xBO_{3-\delta}F_{2\delta}$ (x = 0, 0.25, 0.5, 0.75, and 1.0), which have been synthesized by solid-state method and characterized their structure by X-ray diffraction (XRD). In order to verify the stability of the structure, an electrochemical performance test has also been performed by using the Galvano static charge-discharge measurements.

Poster Presentation : **ANAL.P-317**
Analytical Chemistry
Event Hall THU 11:00~13:00

Development of SF-HF-GC-MS Method for the detection and quantification of benzyl chloride Impurities in a drug product

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A variety of genetically toxic chemical impurities can often be found as by-products during the production of synthetic drugs that are prescribed for the treatment of various diseases such as AIDS, cardiovascular disease, and diabetes. Benzyl chloride is one of the toxic chemicals used in the production process of CinnarizineTM. It is a well-known carcinogen so that the trace amount of them in the drug potentially cause a fatal illness. Therefore, it is important to develop an analytical method that could detect and quantify the benzyl chloride to the low parts-per-billion level. In this study, an analytical method utilizing a solvent-free headspace gas chromatography–mass spectrometry (SF-HS-GC/MS) is developed for screening benzyl chloride within active pharmaceutical ingredients (APIs) and actual products in different product forms such as a capsule and a tablet. The experimental conditions for a solvent free headspace system were optimized using the following parameters: incubation temperature, and time of the sample. The developed SF-HS-GC/MS method was validated in terms of linearity, limit of detection (LOD), limit of quantification (LOQ), accuracy and precision. The calibration curve showed a good linearity from 4 to 200 µg/g with correlation coefficients (R2>0.998). The LOQ of this method was measured to be 4 µg/g which had a signal-to-noise ratio of 10. The accuracy ranged from 90.80 to 118.01% and the precision (%RSD) ranged from 0.34 to 3.67%. The developed SF-HS-GC/MS method can be used as a guideline for screening benzyl chloride in APIs and drug products. This research was supported by a grant (20173MFDS162) from Ministry of Food and Drug Safety in 2022.

Poster Presentation : **ANAL.P-318**

Analytical Chemistry

Event Hall THU 11:00~13:00

Quantitative Analysis of Anti-cancer Drugs and Its Fragmentation Pathways Using Ion Mobility Mass Spectrometry and Tandem Mass Spectrometry

Gyusub Yoon, Sooyeon Chae, MyungKook Son, Dongjoon Im, Dongvin Kwak, Da Gyeong Hyun, Chanju Won, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is one of the representative childhood cancers and a highly heterogeneous disease affected by factors such as age at diagnosis, stage, and tumor biology. Multidrug regimen chemotherapy has been ongoing for high-risk patients and requires customizing to maximize treatment efficiency. To improve the outcomes for neuroblastoma, many research groups and institutes have developed precision medicine (personalized-medicine) using biochemical methods such as genomics and proteomics.Among them, pharmacogenomics and pharmacoproteomics are broader academic fields that identify genes or proteins involved in drug response or disease occurrence. Therefore, It is important to verify pharmacokinetics to develop pharmacogenomics and pharmacoproteomics.In this study, we establish a drug quantitation method for verifying pharmacokinetics using mass spectrometry. Quantitative analysis of Intracellular antidrug was performed using multiple reaction monitoring (MRM) analysis using RPLC-triple quadrupole mass spectrometry. For precise quantitative analysis, the mechanism of fragmentation used in MRM analysis was also investigated. Fragmentation pathways of anticancer drugs were identified using ion mobility mass spectrometry (IM-MS).

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Analytical Chemistry
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Purification of Non-Tagged Recombinant *α*-Synuclein Using Liquid Chromatography Based Separation Methods

Da Gyeong Hyun, Dongjoon Im, MyungKook Son, Sooyeon Chae, Dongvin Kwak, Chanju Won, Gyusub Yoon, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

α-Synuclein aggregates are the pathological hallmarks of synucleinopathies, including Parkinson’s disease and dementia with Lewy bodies. However, there is still no treatment for the synucleinopathies that has been established. To develop a therapeutic strategy, it is crucial to understand the molecular basis of *α*-synuclein aggregation and suppress the pathogenic amyloid aggregate formation. Up to date, as in-human studies are limited, the majority of research findings were based on *in vitro* experiments, with purified recombinant *α*-synuclein used to investigate self-assembly properties. Herein, we developed high-purity recombinant full-length *α*-synuclein expression and purification protocols without affinity tags or linkers. Furthermore, we performed a quality assessment of purified recombinant proteins to confirm the unique properties of *α*-synuclein via biophysical analyses including mass spectrometry-based identification, thioflavin T (ThT) fluorescence assay, and circular dichroism (CD). The compelling results imply that the proposed non-tagged *α*-synuclein preserves its biophysical properties, which can be used in further study to investigate the self-assembly property of *α*-synuclein.

Poster Presentation : **ANAL.P-320**
Analytical Chemistry
Event Hall THU 11:00~13:00

Untargeted Metabolomics of Lettuce (Lactuca sativa) exposed to various chemicals

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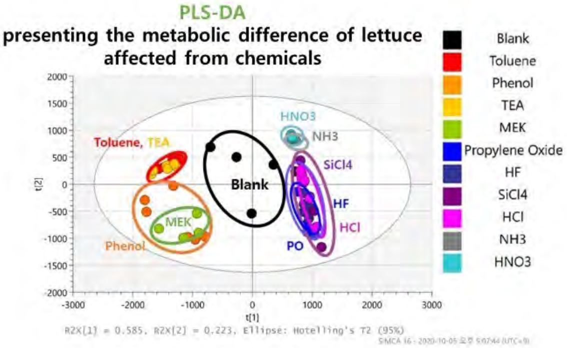
The development of various industrial facilities has led to a drastic increase in the production and consumption of chemicals, increasing the risk of chemical accidents and unauthorized discharge of chemicals to the environment. Hydrogen fluoride leaked in Gumi, North Gyeongsang Province in 2012, causing great damage to crops as well as health damage to residents nearby. At the time of the accident, hydrogen fluoride diffused into the atmosphere and reached crops and soil in nearby farmland. Even though concentration of the hydrogen fluoride in the soil fall behind standard level, some farmers claimed a poor harvest of crops due to chemical accidents and people had been arguing about this problem. To solve this question, the representative chemicals such as toluene, phenol, triethylamine, methyl ethyl ketone, propylene oxide, hydrogen fluoride, silicon tetrachloride, hydrogen chloride, nitric acid, and ammonia were selected for study. A simulation experiment for chemical leak accident was conducted, and the metabolites in the lettuce affected from the chemicals were analyzed using UHPLC-Orbitrap-MS. PLS-DA (Partial Least Squares-Discriminant Analysis) statistical analysis also was applied. The result of this study presented the possibility that contaminated soil, even fallen behind standard level, still exert a hidden effect on the metabolic pathway of crops. The further work for plant stress will be explored.[Acknowledgment]This work was supported by Korea Environment Industry and Technology Institute (KEITI) through the Chemical Accident Prevention Technology Development Project, funded by the Korea Ministry of Environment(MOE) (2020001960001).



PLS-DA

presenting the metabolic difference of lettuce affected from chemicals

Poster Presentation : **ANAL.P-321**

Analytical Chemistry

Event Hall THU 11:00~13:00

Analysis of radioactive material in consumer products using precision gas mass spectrometer

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Some of the products we use daily contain radioactive materials. Among them, tritium (^3H) contained products are less dangerous than other radioactive materials since the lower radiation energy is released when tritium decays. For this reason, tritium is more commonly used in products. The principle that electrons emitted from the decay of tritium reacts with phosphors to emit light is being used in products such as emergency exit signs, watches, and fishing floats. To verify the risk of affecting our health by using these products, a quantitative analysis of tritium contained products is essential. In this study, several product groups containing tritium that imported from abroad (watches, compasses, fishing floats, ear picks, etc.) were analyzed using a Precision Gas Mass Spectrometer (MAT271). We performed the quantitative and qualitative analysis based on the partial pressure of tritium gas and related isotopes (HT, DT, T_2) in the samples. As a result, the amount of gas containing tritium atoms was detected as low as 0.09×10^{-6} g to as high as 6.48×10^{-6} g in one sample, which is the same level of 0.03 GBq to 2.31 GBq. Most of the product groups were shown that values are much lower than the tritium exemption quantity (1 GBq) stipulated by the International Atomic Energy Safety Organization. However, as a result of the analysis, some products were exceeded the exemption quantity.

Poster Presentation : **ANAL.P-322**

Analytical Chemistry

Event Hall THU 11:00~13:00

The SABRE for the polarization of Bis[2-pyridyl(alkyl)]amine

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Signal amplification by reversible exchange (SABRE) is an effective NMR hyperpolarization technique for signal enhancement using *para*hydrogen in an iridium catalyst. To date, monodentate chelated nitrogen analogs have been used primarily as substrates for SABRE because of the limited chelation sites of Ir catalysts with different molecular orientations. To optimize the tridentate chelating ligand, the alkyl chain length was changed according to the optimization of the external magnetic field and the concentration of three different ligands. Since many chemical multi-coordinate complexes in nature have been rarely studied as SABRE substrates, this optimized tridentate chelate ligand structure with SABRE catalyst and polarization transfer from parahydrogen will broaden the scope of hyperpolarizability.

Poster Presentation : **ANAL.P-323**

Analytical Chemistry

Event Hall THU 11:00~13:00

Quantitative analysis of hydrogen isotopes in deuterium and hydrogen gases

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Gas Isotope Metrology team, Korea Research Institute of Standards and Science, Korea

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Stable isotopes of hydrogen include H and deuterium atom (D), and molecules include H_2 (Hydrogen), HD (Hydrogen Deuteride), and D_2 (deuterium). Recently, deuterium has been used instead of hydrogen in industries such as electronics and semiconductors. The diffusion velocity of deuterium is slower than ordinary hydrogen and can improve the stability of the industrial processes of products. Korea exploits more than half of the world market of deuterium and it all relies on import due to lack of industrial facilities to produce suitable deuterium. Many Korean companies are building deuterium production facilities to produce high-purity deuterium. The D_2 is produced by electrolysis of deuterium water (D_2O), the isotopes H_2 and HD exist as impurities with the deuterium gas produced in this process. Without regulation impurities affect the purity of deuterium gas and only high purity gas is required for industrial use. Therefore, determining impurities of D_2 is crucial. In this study, three high purity gases, H_2, D_2 and HD were used to analyze trace amounts of hydrogen isotopes using Precision Gas Mass Spectrometer (MAT271). Hydrogen isotopes present in each gas were quantified using sensitivity values of H_2, HD and D_2 gases. It has been confirmed that there are 300 μmol/mol of HD in H_2, 2500 μmol/mol of HD in D_2, and 5,000 μmol/mol of D_2 in HD. Further, planning to develop certified reference material (CRM) produced by high purity substances, which is for analyzing hydrogen isotopes and used as standard material to quantify the impurities of commercial D_2 gases.

Poster Presentation : **ANAL.P-324**

Analytical Chemistry

Event Hall THU 11:00~13:00

Development of analysis method for high purity nitrogen using GC-FID/Methanizer

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With the rapid development of the technological industry, the need for standard materials and related analysis methods for analyzing high-purity gases and trace impurities in gases that used for manufacturing semiconductors and displays are also increasing. In this study, a certified reference materials (CRM) were developed using the gravimetric method for trace levels of carbon monoxide (CO), carbon dioxide (CO_2), and methane (CH_4) in nitrogen balance. These components possibily exist as impurities of high purity nitrogen. Further analysis method to evaluate the impurities were developed, and CRMs used to determine the purity of high-purity nitrogen. In the developed purity analysis method, the amount-of-substance fraction of impurities in commercial nitrogen was evaluated using the difference in the response area value of CRM obtained from the analysis when ultra-high pure nitrogen and commercial nitrogens were used as carrier gas. Liquid nitrogen and high-purity nitrogen from three different manufacturers were tested as sample nitrogens. For each sample nitrogen, results obtained by our developed purity analysis method and the existing purity analysis methods results were compared, it was confirmed that the amount-of-substance fraction of impurities were consistent within the uncertainty.

Poster Presentation : **ANAL.P-325**

Analytical Chemistry

Event Hall THU 11:00~13:00

Electrochemical discrimination of neurotransmitters using metal-organic framework recognition module on dual-gate based field-effect transistor biosensor

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Qualitative and quantitative analysis of small-molecule such as neurotransmitters using dual-gate field-effect transistor (DGFET) transducers are interferences by the lack of target-specific receptors and Debye shielding in high-ionic-strength media. Here, we report two-dimensional conductive metal-organic frameworks (MOFs) as sensing and recognizing modules of DGFET biosensors for the neurotransmitter. Conductive MOF thin films deposited on the extended gate of DGFET by perceiving catecholamines in physiological solutions, providing readable signals even at a concentration of ~2nM. Adsorption of analytes inside the MOFs induces identical voltage shifts regardless of the ionic strength of the sensing media, addressing the Debye shielding effect. As a recognition module, a cross-reactive MOF sensor array discriminates chemically similar neurotransmitters by means of differentiated adsorption, which is attributed to the tunable physicochemical features of MOFs, such as pore size and surface properties. Furthermore, we demonstrate simultaneous discrimination capability under the interference of biologically relevant substances and artificial cerebrospinal fluid.

Poster Presentation : **ANAL.P-326**

Analytical Chemistry

Event Hall THU 11:00~13:00

Conformation Ensembles of Pathologically Disordered Proteins

Dongjoon Im, MyungKook Son, Da Gyeong Hyun, Sooyeon Chae, Chanju Won, Gyusub Yoon, Dongvin Kwak, Hugh I. Kim[*]

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As the number of people suffering from neurodegenerative diseases, such as dementia, grows, they have become a serious social burden. Nevertheless, the majority of dementia treatments aim to alleviate symptoms in the short term. Understanding the nature of a protein identified as a pathogen is required for developing a more effective treatment. However, intrinsically disordered proteins, which have been identified as the cause of dementia, can exist in a heterogeneous states and do not have a specific favorable structure, particularly at the early stage of aggregation. As a result, an analysis method capable of comprehensively analyzing various structure ensembles in which proteins may exist is required. Herein, we investigated the conformation ensemble of amyloid-β (1-42) and tau, which are closely related to the pathological hallmarks in Alzheimer's disease using replica exchange molecular dynamics simulations. We identified protein interactions that play an active role on the early stages of amyloid aggregation by *in silico* analyses. Furthermore, combined with an interdisciplinary biophysical approach, we observed how the theoretically identified structural properties were expressed *in vitro*. Overall, this methodology, based on the structural dynamics of pathologically disordered proteins, could be applied to theoretically predict and inhibit self-assembly properties.

Poster Presentation : **ANAL.P-327**
Analytical Chemistry
Event Hall THU 11:00~13:00

The pharmaceutical and biomimetic models with quantitative analysis for precision medicine

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Precision medicine for solid cancer is targeted therapy based on scientific evidence such as pharmaceutic factor, gene, protein, and metabolite. Therefore, investigating accurate scientific evidence is critical for providing precision medicine for each patient. In general, scientific evidence was firstly investigated in the laboratory cell-based screening model. However, this model does not consider pharmacokinetics, structures, and microenvironments of solid cancer. Consequently, drugs efficacy or targeting biomarkers have shown discriminated results in clinical tests or therapy. Therefore, it is necessary to discover reliable biomarkers using pharmaceutical and biomimetic models at the pre-clinical level.Several clinical tests showed that the multidrug regimens have synergistic drug efficacy. However, the specific mechanisms of this effect and appropriate combinations of drugs are still ambiguous due to challenges at mimicry of pharmacokinetics and the tumor microenvironment at the laboratory level. We have constructed the pharmaceutical and biomimetic models with our Artificial Circulatory System for Tumoroid (ACST). Pharmacokinetic software, and microfluidic systems were used for the ACST systems. The results obtained from cutting-edge analysis techniques, including mass spectrometry (MS), ion mobility mass spectrometry (IM-MS), and spectroscopy, provided detailed drug action mechanisms based on the quantitative analyses.

Poster Presentation : **ANAL.P-328**

Analytical Chemistry

Event Hall THU 11:00~13:00

Synthesis of Hollow mesoporous carbon spheres (HMCSs) incorporated with gold nanoclusters

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Electrochemiluminescence (ECL) is an electrochemical process in which species generated at electrodes undergo high energy electron transfer reactions to form excited states that emit light. Recent studies including ours demonstrated analytical benefits of Au nanoclusters as a stable and biocompatible ECL emitter. In this study, we synthesized hollow mesoporous carbon spheres (HMCSs) incorporating glutathione-stabilized Au nanoclusters (Au NCs) within mesoporous shell of HMCSs. We envision the HMCSs incorporating Au NCs as an efficient ECL emitter platform exhibiting amplified ECL of the Au NCs by confining the NCs within the conductive mesoporous shell of HMCSs.

Poster Presentation : **ANAL.P-329**

Analytical Chemistry

Event Hall THU 11:00~13:00

Photoluminescence and electrochemiluminescence properties of Au(I)-glutathione complexes depending on pH conditions

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Department of Chemistry, Kyung Hee University, Korea

Electrochemiluminescence (ECL) is an electrochemical phenomenon in which electrochemically-generated species undergo electron transfer reactions to produce excited species emitting light at electrodes. The ECL has the advantages of high sensitivity and low background noise, and thus has been used in various fields such as biosensing, clinical diagnosis, environmental monitoring. In this study, we synthesized Au(I)-glutathione complexes under different pH conditions, then compared their ECL properties as well as photoluminescence (PL) properties. Glutathione is a tripeptide having two carboxyl groups and one amine group. As pH conditions change, Au(I)-glutathione complexes undergo a reversible assembly-disassembly process due to the functional groups of glutathione. Therefore, the aggregation extent of the Au(I)-glutathione complexes varies depending on the pH conditions. Because the aggregation of the Au(I)-glutathione complexes results in the aggregation-induced emission (AIE) of the complexes, we demonstrated different ECL and PL behaviors of the Au(I)-glutathione complexes depending on the pH conditions.

Poster Presentation : **ANAL.P-330**

Analytical Chemistry

Event Hall THU 11:00~13:00

[Withdrawal] Condensation effect caused by phase change of insulin due to PEG

Dongvin Kwak, Hugh I. Kim*, Sooyeon Chae, MyungKook Son, Dongjoon Im, Da Gyeong Hyun, Chanju Won, Gyusub Yoon

Department of Chemistry, Korea University, Korea

- Withdrawal -

Poster Presentation : **ANAL.P-331**

Analytical Chemistry

Event Hall THU 11:00~13:00

A study on overall migration from plastic packaging into cosmetic simulants

Juyoung Han, Neulhwi Yeo, Doyoon Park, Seok Yoon Kim, Hyo-Yeon Yu, Jieun Min[1], Somi Chu[1], Sangdoo Ahn[*]

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In plastic packaging materials that directly contact products (food, pharmaceuticals, cosmetics, and etc.) interactions such as permeation, adsorption, and migration may occur due to contact with internal substances. In particular, migration is the transfer of substances from plastic packaging to products, and some of the substances transmitted can potentially have side effects on human health. In this study, overall migration were studied from LLDPE, PCTG, and PCTA packaging into cosmetic simulants such as ethyl alcohol, acetic acid, and ammonia solution through incubation at 40°C for 10 days according to the EU's Food Plastics Compliance Test Standard. Qualitative analysis was also performed using gas chromatography to specify the migration material.

Poster Presentation : **ANAL.P-332**

Analytical Chemistry

Event Hall THU 11:00~13:00

MRM-based prediction of disease subtypes: A case of pancreatic ductal adenocarcinoma

Jiwon Hong, Seunghoon Back, Dowoon Nam, Jingi Bae, Hokeun Kim, Su-Jin Kim, Chaewon Kang, Kwon Hee Bok, Hye-Kyeong Kwon, Sang-Won Lee*

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Identification of disease subtypes can facilitate tailoring therapeutic strategies. At a glance, progression of a disease may seem similiar across all patients, yet the underlying mechanism at molecular level can differ greatly. Applying appropriate therapies to target the right progression pathway would enable patients to have optimal therapeutic benefits with minimized side effects. In order to optimize the therapeutic option, it is crucial to be able to identify disease subtypes promptly with high certainty. Here, a MRM-based subtype prediction method is introduced with its application to pancreatic ductal adenocarcinoma (PDAC), one of the diseases with lowest average 5-year survival rate. More than 90% of the patients do not show response to surgery or chemotherapy, which necessitates a way to tailor appropriate therapeutic options. An extensive proteogenomic characterization identified 6 subtypes of PDAC and subtype specific signature peptides. Based on pathway enrichment and network analyses, as well as the adequacy for MRM, a set of subtype specific peptides were chosen for MRM-based subtype identification. These peptides were stable isotope labeled (SIL), purified, quantified respectively then mixed together to create a PDAC subtype identification SIL peptide mixture for spiking in MRM validation experiments. From the MRM-quantified endogenous peptide amounts, key subtype signature peptides were extracted and taken to build a PLS-DA model with an average 88.9% accuracy and AUC of 0.905 in all 6 subtypes. We plan to examine the correlation between survival rates and the deduced subtypes from the prediction model to assess the value of the PDAC subtype identification technology (PDAC-SIT) for clinical trials of drug candidates as a predictive enrichment strategy.

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Poster Presentation : **ANAL.P-333**

Analytical Chemistry

Event Hall THU 11:00~13:00

Influence of plasma treatment on AuNRs immobilized on ITO surfaces

Ji Won Ha*, Mukunthan Ramasamy

Department of Chemistry, University of Ulsan, Korea

Localized surface plasmon resonance (LSPR) is a unique property associated with certain metallic nanomaterials (e.g., Au, Ag, Cu). LSPR is a collective oscillation of conduction band free electrons in metallic nanostructures due to interactions with light. The LSPR spectrum of plasmonic nanoparticles (eg. Au, Ag, Cu) is influenced by the size, shape, composition, and change in dielectric properties of the surrounding medium (refractive index). Gold nanoparticles (AuNPs) have been considered in this work because of their broadly tunable size, shape, and structure-dependent optical properties, the easy possibility of surface modifications by biological and organic molecules, biocompatibility, and photostability. Plasma, the fourth state of matter, is a partially ionized gas consisting of electrons, ions, and neutral atoms/ molecules. Radiofrequency (RF) plasma, a nonthermal plasma (the gas temperature is as low as room temperature), is often used to remove surface capping material and to change the morphology of metallic nanoparticles (NPs). In this study, we discuss the spectral, structural, and electrochemical behavior of AuNRs immobilized of ITO for various plasma exposure times by dark-field (DF) microscopy and spectroscopy, scanning electron microscopy (SEM), and cyclic voltammetry (CV). Single gold nanorods (AuNRs) of considerable size were immobilized on the ITO surface and have been subjected to various plasma exposure times. We analyze here the LSPR linewidth variations of scattering spectra, effect in aspect ratio (AR) and morphology of AuNRs from SEM image analysis, and possible facet modification of AuNRs from CV analysis as a function of plasma exposure time.

Poster Presentation : **ANAL.P-334**

Analytical Chemistry

Event Hall THU 11:00~13:00

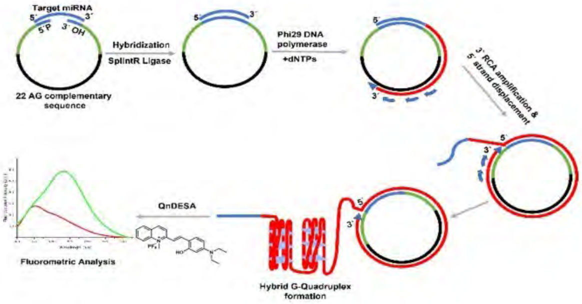
Highly sensitive, selective, and rapid detection of miRNA-21 using an RCA/G-quadruplex/QnDESA probing system

Tasnima Alam Asa, **Young Jun Seo**[1,*]

Chemistry, Jeonbuk National University, Korea

[1]*Department of Chemistry, Jeonbuk National University, Korea*

In this study, we developed a very simple and rapid miRNA 21 detection system using a novel quinolinium diethylamino salicylaldehyde (QnDESA) probe for sensing the 22AG hybrid G-quadruplex with a single-step rolling circle amplification (RCA) reaction. We synthesized a circular DNA padlock template containing a sequence complementary to the 22AG hybrid G-quadruplex, used SplintR ligase to ensure perfect hybridization with miRNA 21, applied this circular DNA and phi-29 DNA polymerase for tandem amplification of the 22AG hybrid G-quadruplex sequence, and then probed the product using QnDESA. This combination of RCA-G-quadruplex and QnDESA allowed the rapid (1 h) and simple one-pot detection of miRNA 21 based on a change in fluorescence. In addition, this system displayed high sensitivity (limit of detection: 1.37 fM) and selectivity. This probing system should also be useful for identifying a diverse range of DNA- and RNA-based biomarkers.



Poster Presentation : **ANAL.P-335**

Analytical Chemistry

Event Hall THU 11:00~13:00

Wide-band PRM : Novel quantification method for large-scale global targeting with highly reliable quantitative information

Dowoon Nam, MinYoung Ji, Hokeun Kim[1], Sang-Won Lee[1,*]

Korea University, Korea
[1]*Department of Chemistry, Korea University, Korea*

Mass spectrometry (MS)-based quantitative proteomic methods have been widely used for protein biomarker validation. Recent advances in mass spectrometers and liquid chromatography allowed various ways of parallel reaction monitoring (PRM) technique to be developed for more accurate quantitative information or to enlarge target lists. However, in case of accuracy, conventional PRM technique produces quantitative information of labeled peptide and endogenous peptide separately from each tandem scans. The targeting peptides, both labeled peptide and endogenous peptide, are listed in MS method altogether, so each peptides are scanned separately. Calculating profile area from two different scans to obtain ratio between labeled peptide and corresponding endogenous peptide can provide inaccurate quantitative information. In order to avoid such discrepancy between scans, we employed novel quantification method using wide isolation window to capture both labeled peptide and endogenous peptide in single tandem scan. By using wide-band PRM method coupled with high resolution dual online-ultrahigh pressure liquid chromatography (DO-UHPLC) system, we were able to quantify 150 targeted peptides from pancreatic ductal adenocarcinoma(PDAC) sample in single experiment.

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Poster Presentation : **ANAL.P-336**

Analytical Chemistry

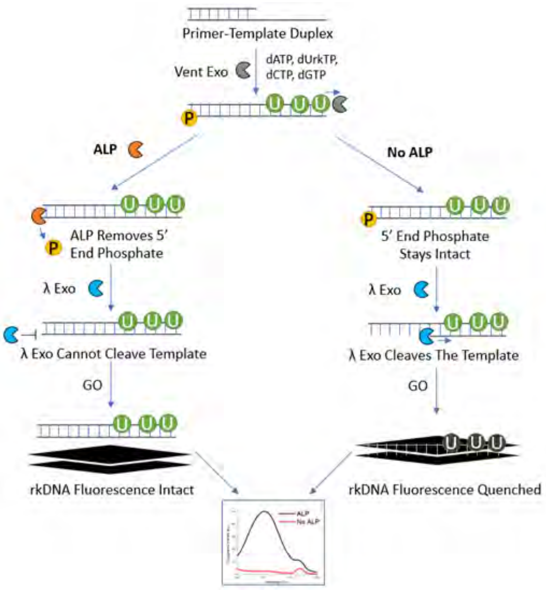
Event Hall THU 11:00~13:00

Unnatural Nucleotide–Based rkDNA Probe Combined with Graphene Oxide for Detection of Alkaline Phosphatase Activity

Kazi Morshed Alom, Young Jun Seo*

Department of Chemistry, Jeonbuk National University, Korea

We have developed a fluorescent double-stranded DNA, incorporating an unnatural dU^{rk} nucleotide, that we used as a probe for the detection of alkaline phosphatase (ALP) based on enzymatic cleavage of the non-fluorescent complementary strand. Primer extension performed using the unnatural nucleotide triphosphate $dU^{rk}TP$ and the natural deoxynucleotide triphosphates dATP, dCTP, and dGTP provided a simple fluorescent DNA strand that hybridized with the 5´-monophosphate non-fluorescent complementary strand. When applying the 5´-phosphate recognition and cleavage properties of lambda exonuclease (λ-exo), this probe could bind to graphene oxide (GO) and quench the fluorescence (in the absence of ALP) or not bind to GO and retain its fluorescence (in the presence of ALP). We obtained strongly fluorescent DNA strands through simple incorporation of multiple A sites in the complementary sequence, thereby increasing the number of dU^{rk} residues during primer extension. This unnatural nucleotide–based rkDNA probing system exhibited high fluorescence differentiation for discriminating the status of ALP. This rkDNA-GO probing system appears to be a promising tool for monitoring the activity of disease-associated enzymes.


Primer-Template Duplex
Vent Exo
dATP, dUrkTP,
dCTP, dGTP
P
U U U
ALP
No ALP
ALP Removes 5′
End Phosphate
5′ End Phosphate
Stays Intact
λ Exo
λ Exo Cannot Cleave Template
λ Exo Cleaves The Template
GO
rkDNA Fluorescence Intact
rkDNA Fluorescence Quenched
ALP
No ALP

Poster Presentation : **ANAL.P-337**

Analytical Chemistry

Event Hall THU 11:00~13:00

Au/Pd Bimetallic Core-Shell Structures for Plasmon-Mediated Photocatalyst

Suhyun Kim, Jeong-Wook Oh[1,*]

Chemistry, Hankuk University of Foreign Studies, Korea

[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Palladium is widely used in various chemical reactions due to its high catalytic activity characteristics.Although metal nanoparticles have attracted much interest in photocatalytic reactions, palladium exhibitslower plasmonic properties than coinage metals such as Au, Ag, and Cu. We developed Au/Pd bimetalliccore-shell structure for a highly efficient plasmon-mediated photocatalyst. After the Au/Pd nanostructureswere synthesized with controlling the thickness of the Pd shell, they were used as photocatalysts forreducing 4-Nitrothiophenol to 4-Aminobenzenethiol, which were observed by in-situ RamanSpectroscopy. We demonstrated a synergistic effect of Au/Pd nanostructures combining the inherentcatalytic effect of palladium with the plasmonic effect of Au nanoparticles.

Poster Presentation : **ANAL.P-338**

Analytical Chemistry

Event Hall THU 11:00~13:00

Absolute Quantification of Glycans using Unlabeled Standard and Isotope-labeled Analytes by Mass Spectrometry

Jihee Yun, Jae-Min Lim*

Department of Chemistry, Changwon National University, Korea

Protein glycosylation is one of the most common post-translational modifications (PTMs). Glycans not only directly participate in cell development and cell differentiation, but also provide genetic or pathological information. It is important to understand changes in glycan expression levels to identify correlations with glycan function and disease. Therefore, many relative quantification techniques have been developed through isotope labeling strategies based on mass spectrometry. However, absolute quantification techniques suffer from many difficulties due to the synthesis of isotopically labeled standards. In this study, Quantitative Analysis using Unlabeled Standard and Isotope-labeled Analytes (QAUSIA) is presented to realize absolute quantification of glycan. We successfully labeled glycans in yeast using 1-$^{13}C_1$ glucose based on Metabolic Isotope Labeling of Polysaccharides with Isotopic Glucose (MILPIG) strategy for isotopic labeling of analytes. Then, it was combined with an unlabeled internal standard to obtain a calibration curve showing excellent linearity and reproducibility based on mass spectrometry. In addition, the applicability in biological conditions was confirmed using tunicamycin, a glycosylation inhibitor, through two internal standards. In conclusion, we indicate that QAUSIA is relevant for establishing a simple, fast, and effective absolute quantitative assay for analyzing absolute glycan information in disease.

Poster Presentation : **ANAL.P-339**
Analytical Chemistry
Event Hall THU 11:00~13:00

Artificial intelligence analysis of 1H NMR spectra for discriminating the geographical origin of Asian red pepper powder

Sangdoo Ahn*, Byung Hoon Yun, Hyeong Min Kim, Hyo-Yeon Yu

Department of Chemistry, Chung-Ang University, Korea

The purpose of this study is to develop a method to identify the geographical origin of Asian red pepper powder based on artificial intelligence analysis of 1H NMR spectrum. A support vector machine (SVM) and convolutional neural network (CNN) deep learning models were employed to analyze the 600 MHz 1H NMR spectral data of 300 red pepper powder samples, 100 each from Korea, China, and Vietnam respectively, distributed in Korea. Since the 1H NMR spectrum of red pepper powder appears in a very complex pattern due to the various metabolites of red pepper powder, the spectrum was divided into several parts and analyzed to compare the identification accuracy according to the spectrum range. The optimized SVM and CNN deep learning models showed higher accuracy in discriminating the geographical origin of red pepper powders than the data processing methods using statistical techniques. These results demonstrated the feasibility that artificial intelligence techniques can be effectively used to discriminate NMR spectra of foods, which are difficult to completely distinguish with conventional statistical means.

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Poster Presentation : **ANAL.P-340**

Analytical Chemistry

Event Hall THU 11:00~13:00

A study on Forensic Questioned Document Dating through GC/MS analysis of 2-Phenoxyethanol in black ballpoint pen ink

SangJae Oh, Seung-Jin Ryu[1,*]

Korean National Police University, Korea

[1]*Department of Law,Forensic Science Research Center, Korean National Police University, Korea*

In order to analyze the dating of the Questioned Document, 2-Phenoxyethanol in black ballpoint pen ink was selected as an indicator and analyzed as GC/MS equipped with polar column. Black ballpoint pen samples prepared from 1 month to 20 months ago were collected using micro-punch, heated, extracted with a solvent(methanol), and analyzed, and m-cresol was used as the internal standard material. The result showed a tendency to decrease in detection as the time of writing the black ballpoint pen samples old. The amount of detection was calculated in various ratios, but in samples with a time of 3 months or more, it was difficult to specify the time of writing. It is expected that this can be improved by increasing the discrimination power of each sample through the improvement of the pretreatment method of the sample.

Poster Presentation : **ANAL.P-341**
Analytical Chemistry
Event Hall THU 11:00~13:00

A study on Forensic Questioned Document Dating through GC/MS analysis of derivative 2-Phenoxyethanol in black ballpoint pen ink

SangJae Oh, Seung-Jin Ryu[1,*]

Korean National Police University, Korea
[1]*Department of Law,Forensic Science Research Center, Korean National Police University, Korea*

In order to analyze the dating of the Questioned Document, 2-Phenoxyethanol in black ballpoint pen ink was selected as an indicator material, which was derivatively analyzed with GC/MS equipped with a non-polar column. Black ballpoint pen samples prepared from 1 month to 20 months ago were collected using micro-punch, heated, then analyzed by extracting solvent (Methanol) and derivatives with BSTFA reagents, and m-cresol was used as an internal standard. The result showed a tendency to decrease the detection amount as the black ballpoint samples were written longer, and in particular, ballpoint samples prepared within 11 months showed a tendency to decrease classifiable by section in the first extraction detection amount/second extraction detection amount ratio. It is expected that an analysis technique that is more distinctive and has credibility and reproducibility can be established through improvement of the pretreatment techniques.

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Poster Presentation : **ANAL.P-342**

Analytical Chemistry

Event Hall THU 11:00~13:00

Fully automated Dual online reverse-phase liquid chromatography for effective and high throughput proteome analysis

Chaewon Kang, Soo Hyun Jung, Sang-Won Lee*

Department of Chemistry, Korea University, Korea

One of the ultimate goals of clinical proteomics is to find the biological marker molecules. After the discovery, these potential protein biomarkers would be verified and validated on a larger scale of sample size. Therefore, the large number of samples requires a fast method using a short gradient reverse-phase liquid chromatography with no dead time between experiments. In this study, a simple dual online reverse-phase liquid chromatography system has been developed for high-throughput analyses. This simple system apply two additional switching valves (2 position 4 port valve) on a single LC system utilizing two binary pumps. This system is fully automated and offers many advantages such as high duty cycle, high separation resolution, and high intra/inter column reproducibility. In contrast with a single LC system, the dual online reverse-phase liquid chromatography system use two analytical columns alternatively and independently to remove dead time for sample injection, column wash and equilibration. As a result, this system provides an increase in experimental throughput by two folds, while keeping the reproducibility between two analytical columns. This simple system was applied for the MRM experiments and optimized 10 minutes gradient to perform 144 analyses per day. Therefore, this system is ideal for high-throughput MRM experiments, involving a large cohort sample.

Poster Presentation : **ANAL.P-343**

Analytical Chemistry

Event Hall THU 11:00~13:00

Engineering Oxidase-Mimicking Activity of Dendrimer-Encapsulated Pt Nanoparticles

Hyein Lee, Joohoon Kim*

Department of Chemistry, Kyung Hee University, Korea

Here, we report the engineered oxidase-mimetic activity of dendrimer-encapsulated Pt nanoparticles (Pt DENs) by precisely controlling their sizes in the diameter range of 1.8 – 3.1 nm. Using a dendrimer-template method, we synthesized five different Pt DENs (i.e., Pt_{200}, Pt_{220}, Pt_{550}, Pt_{880}, and Pt_{1320} DENs) having sizes in the range of 1.8 – 3.1 nm. The as-synthesized Pt DENs exhibit oxidase-mimetic activity for the oxidation of Amplex Red to form fluorescent resorufin in the presence of oxygen. Mechanistic study indicates that Pt DENs catalyzed activation of dissolved oxygen to generate reactive oxygen species (ROSs) (i.e., $OH^{\bullet}$, $O_2^{\bullet -}$, and $^1O_2$) and the ROSs are responsible for the oxidation of Amplex Red to resorufin. The enzyme-mimetic activity of Pt DEN was tunable by changing the size of Pt nanoparticles, and especially up to Pt_{1320} DENs with a diameter of 3.1 nm. The oxidase-like activity of Pt DENs tends to increase as their size increased. Interestingly, Pt_{1320} DENs exhibit a ~117-fold higher catalytic activity compared to Pt_{200} DENs, although they were only 1.2 nm larger in diameter than Pt_{200} DENs. We envision that this study can provide insights into the design of artificial enzymes having excellent performance.

Poster Presentation : **ANAL.P-344**
Analytical Chemistry
Event Hall THU 11:00~13:00

Development of Droplet-based Analytical Platform for Real-time, High-throughput and Absolute Quantification

Sunghyun Ki, Dong-Ku Kang[1,*]

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[1]*Department of Chemistry, Incheon National University, Korea*

Droplet microfluidics (DMF) has been developed and used as digital assays for accurate and absolute quantification of biological markers such as viruses, bacteria and nucleic acids. Currently, representative droplets analysis approaches include one-dimensional channel detection and two-dimensional area detection. However, these approaches have the disadvantage of expensive optic system and end-point detection, and require a high-throughput and rapid assay time. To avoid complex and expensive optic system as a detector, CMOS image sensor and smartphones have been integrated with DMF to analysis droplets. Here, we introduce a droplets analysis approach for multiplexing, absolute quantification and high-throughput. In this approach, DMF was integrated with wide-field imaging system (WIS) for the accurate and precise digital quantification of droplets within a single image. To setup the WIS, 100 mm macro lens and 50.6-megapixel CMOS image sensor were used to image droplets, and droplet images were identified with MATLAB-based homemade software that simultaneously analyzes eight individual colors for multiplexed, real-time monitoring and absolute quantification. Using this platform, it can be used for identification of each eight different targets (colors) and sensitivity was characterized as low as 0.01%. The WIS allowed imaging area from a minimum of 11.48 cm2 to a maximum of 201.84 cm2 and theoretical number of droplets, that can be analyzed, were calculated from 5.84x105 to 1.03x107 droplets when droplets are generated at 50 μm in a diameter. This platform technology will provide a tool for high-throughput, absolute and real-time quantification of droplets that can be used as a tool such as high-throughput digital PCR and digital ELISA for accurate diagnostics.

Poster Presentation : **ANAL.P-345**

Analytical Chemistry

Event Hall THU 11:00~13:00

Quantitation and Speciation of Inorganic Arsenic in a biological sample by Capillary Ion Chromatography coupled with Inductively Coupled Plasma Mass Spectrometry

Seon-jin Yang, Sang-Ho Nam*, Yonghoon Lee

Department of Chemistry, Mokpo National University, Korea

Arsenic is a nonmetallic element known to be toxic to the human body, and when it accumulates in our bodies through food and drinking water can cause serious illness. Since arsenic has different toxicity depending on its chemical form, it is important to measure not only the element itself but also the arsenic species. For the separation of arsenic species, cation and anion exchange separation columns are used, where the sample loop volume used is usually 100-200 μL. However, the amount of sample actually required is at least 0.5 to 1 mL or more. In this case, it is difficult to apply to limited samples such as clinical and biological samples. Therefore, in this study, a method for separating arsenic species was developed by using a capillary ion exchange column with a sample loop of 5 μL to reduce the sample volume. The separated arsenic was measured by inductively coupled plasma mass spectrometry (ICP-MS). For inorganic arsenic, a linear calibration curve from 0.5 μg/kg to 25 μg/kg was obtained, and the correlation coefficient was 0.9999. Using the developed method, the rate of recovery of inorganic arsenic from standard certified substances in water was about 100%, and the rate of recovery of inorganic arsenic from urine standard certified substances with complex substrates was about 121%.

Poster Presentation : **ANAL.P-346**

Analytical Chemistry

Event Hall THU 11:00~13:00

Identification and characterization of enzymes that degrade polystyrene from insect

Hwicheol Shin, Dong-Ku Kang[1,*]

Chemisty, Incheon National University, Korea

[1]*Department of Chemistry, Incheon National University, Korea*

The term Plastic is a High-molecular-carbon-polymers that do not break down in a natural condition by biological processes. It has been extensively worldwide used and its' accumulation has become a worldwide concern. In this study, various insects that degrade plastic were discovered and the plastic degrading enzymes possessed by insects were investigated. The selected target species were Galleria mellonella, Tenebrio molitor Linnaeus and Plodia interpunctella that were collected from national environment. For the target species, we provided plastics that emit the most, such as polyethylene (PE) and polystyrene (PS). It was confirmed that Tenebrio molitor larvae feed on PS rapidly, and the occurrence of digestive enzymes according to the presence or absence of intestinal microorganisms was compared through DNA analysis. Through this, it was confirmed that the intestinal microorganisms and the intestinal digestive enzymes of insects are also involved in the degradation of plastics.

Poster Presentation : **ANAL.P-347**
Analytical Chemistry
Event Hall THU 11:00~13:00

Studying Lipid Changes in the *Drosophila* Head of Amyotrophic Lateral Sclerosis Model by Time-of-Flight Secondary Ion Mass Image Spectrometry

Jin Gyeong Son*, Hyun Kyong Shon[1], Tae geol Lee[2,*]

Bioimaging team, Korea Research Institute of Standards and Science, Korea
[1]*Korea Research Institute of Standards and Science, Korea*
[2]*Center for Nano-Bio Measurement, Korea Research Institute of Standards and Science, Korea*

Lipid profile studies on complex nervous systems have been mainly done by extraction and LC MS based analysis. However, there is a limit to obtaining spatiotemporal information on tissue samples. By combining Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and genetic techniques, we studied the pathogenic effects of altered lipid profiles in the context of amyotrophic lateral sclerosis (ALS), one of the typical neurodegenerative illnesses. For lipid identification, hybrid Orbitrap–SIMS instrument was employed (Hybrid SIMS, IONTOF GmbH Muenster, Germany), using a 20 keV Ar_{3000}^+ cluster primary ion beam. The PCA was employed to differentiate changes in WT and ALS brain tissues over day 1, 3, 5 and 9. We discovered that at the early stages (5 days) of illness progression, the quantity of fatty acids (FAs) and diacylglycerols (DAGs) were raised in the brains of Drosophila over-expressing enlarged G_4C_2 hexanucleotides, the most prevalent genetic cause of ALS at the early stages (5-day) of disease progression prior to motor symptoms.

Poster Presentation : **ANAL.P-348**

Analytical Chemistry

Event Hall THU 11:00~13:00

ToF-SIMS Mass Imaging Analysis Study of 6-OHDA-Induced Parkinson's Mouse Model

Hyun Kyong Shon, Sun Young Lee, Tae geol Lee[1,*], Jin Gyeong Son[2,*]

Korea Research Institute of Standards and Science, Korea

[1]*Center for Nano-Bio Measurement, Korea Research Institute of Standards and Science, Korea*

[2]*Bioimaging team, Korea Research Institute of Standards and Science, Korea*

Parkinson's disease is a movement illness that affects the nerve system. The loss of dopaminergic neurons from the substantia nigra (SN) that project to the dorsal striatum is a hallmark of Parkinson's disease (PD) (caudate-putamen). Using a unilateral 6-hydroxydopamine rat model of Parkinson's disease, we tried to mass image analysis profile the disease-related candidate lipids by comparing the difference between the brain lesion region and the normal region using time-of-flight secondary ion mass spectrometry (ToF-SIMS). In addition, although it is not an actual drug injection region, we tried to discover a region showing a difference in the left and right hemispheres and identify candidate molecules contributing to Parkinson's disease. As a result of the analysis, the change in the surrounding area was clear rather than the SN area where the actual drug was injected. In addition, mass image analysis has significance as a method of confirming overall changes in the brain caused by neuronal cell death and dopaminergic signal degradation.

Poster Presentation : **ANAL.P-349**

Analytical Chemistry

Event Hall THU 11:00~13:00

Copper/Arsenite complexed Fenton-like Nanoparticles for Cancer Therapy

KyungKwan Lee, Hongki Kim[1,*]

Hazards Monitoring Bionano Research Center, Korea Research Institute of Bioscience & Biotechno, Korea

[1]*Department of Chemistry, Kongju National University, Korea*

We report copper(II) arsenite-encapsulated ferritin nanoparticles (CuAS-Fn) as a class of Fenton-like reaction-performing oxidative stress-amplifying agents for cancer therapy. Ferritin (Fn) nanoparticles capable of trapping metal species in the core were expressed in E-coli. CuAs-Fn were fabricated through metal-peptide chelation-based formation of the CuAs complex on the core domain of Fn. In physiological pH, CuAs-Fn maintains structural stability, whereas the CuAS-complex was ionized to release arsenite and copper ions at endosomal pH conditions. Thus, the CuAs-Fn can simultaneously release H2O2-generating drugs (arsenite) and Fenton-like catalysts (Cu+) in cancer cells, which synergistically promoted the level of highly cytotoxic hydroxyl radicals. This study demonstrates the tremendous potential of CuAs-complexed Fenton-like nanoparticles as a new theranostic platform with high precision and efficacy for cancer treatment.

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Poster Presentation : **ANAL.P-350**

Analytical Chemistry

Event Hall THU 11:00~13:00

Environmental monitoring of fine dust & virus using spark-induced plasma emission

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As of March 2020, the coronavirus developed in Wuhan has officially been classified as a pandemic. Coronavirus has long been known to be non-infectious when airborne; however, studies are starting to show that several viruses can, in fact, infect through airborne transmission and can remain airborne for significant periods of time.Furthermore, fine dust air pollution caused by various sources such as heavy metals in industrial complexes and ammonia gas in agricultural complexes is a critical problem for modern people wanting to live a healthy life. Accordingly, the study attempts to introduce an innovative and effective technique for real-time monitoring of toxic components in fine dust and virus using plasma emission. Therefore, in this study, an experiment was performed to detect the concentration and characteristics of air transmission in fine dust, and viruses through the utilization of a spark-induced plasma spectroscopic device capable of real-time analysis. Variations in the results of plasma spectroscopy in specific atomic signals were detected through experiments using various types of fine dust sources and viruses. Then, the risk of air propagation was quantitatively detected by changing the fine dust and virus concentration according to traveled distance and measurement time. Also, the densely connected convolutional networks (DenseNet) are used with measured plasma emission to identify PM sources. Consequently, this study provides a benchmark of real-time detection and environmental monitoring of particulate matter in the air.

Poster Presentation : **ANAL.P-351**

Analytical Chemistry

Event Hall THU 11:00~13:00

Fe-Based Mesoporous Nanostructures for Electrochemical Conversion and Storage of Energy

Lemma Teshome Tufa, **Jaebeom Lee***

Chemistry, Chungnam National University, Korea

Decarbonization of the global energy system requires a coordinated effort towards disruptive technology of renewable energy conversion and storage (ECS) that can be potential to secure and diversify energy systems by increasing efficiency of conversion and storage of intermittent energy sources. Porous nanostructures have been newly reported as a promising class of most effective materials for (ECS) because of their unique advantages in terms of large surface-to-volume ratios, surface permeability, and void spaces. These offer abundant active sites for electrochemical activities by shortening the pathway of mass/charge transport. Particularly, Fe-based mesoporous nanostructures (mp-FeNSs) have been recently fascinating. Iron is a principal active center in nanocomposites and has high industrial suitability for next-generation technology owing to its environment friendliness, abundance, and low cost. Crucial technical advances related to Fe-based mesoporous nanostructures are discussed in terms of synthesis, structural design strategy, and ECS applications such as water electrocatalysis, Li-ion batteries, and supercapacitors.

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Poster Presentation : **ANAL.P-352**
Analytical Chemistry
Event Hall THU 11:00~13:00

Analysis of Volatile Organic Compounds Produced in Non-degradable and Biodegradable Plastics during Incineration

Min Jang, Hyemin Yang, Jeyoung Park[1,*]

Center for Bio-based Chemistry, Korea Research Institute of Chemical Technology, Korea
[1]*Center for Biochemistry, Korea Research Institute of Chemical Technology, Korea*

The conventional plastics undoubtedly flourished our lives and society. However, disposal of the non-degradable accumulated plastics became globally serious environmental problems. As an alternative, incineration of them are still being carried out to dispose them, but it may cause toxic volatile organic compounds (VOCs) emission. In order to solve the problems, biodegradable plastics have been developed and started to be commercialized recently. Nevertheless, biodegradable plastics are still discarded indiscreetly and mixed with the conventional non-degradable plastics due to lack of policy and limited market share, thus they can be incinerated together. Previously, studies regarding VOCs from polymers had rarely explored the level of toxicants during the combustion process. This study, for the first time, aims qualitative and quantitative analysis on VOCs emitted from both non-degradable and biodegradable plastics during combustion using gas chromatography mass spectrometry. As a result, the levels of VOCs in non-degradable poly(vinyl chloride) and poly(ethylene terephthalate) were approximately >100 times higher than biodegradable polyhydroxyalkanoate and poly(lactic acid). Interestingly, 1,3-butadiene accounts for the highest concentration among VOCs in both non-degradable and biodegradable plastics owing to the presence of butylene repeating unit. Exemplary case of gas barrier films for food packaging purpose, non-degradable aluminum-coated multi-layered film emits more of VOCs rather than biodegradable nanocellulose/nanochitin-coated film. Nevertheless, incineration of biodegradable plastics cannot be an ultimate solution because VOCs are still emitted when incompletely combusted. This study encourages the necessities of research on more diverse combustion conditions for various plastics and related discussion on the fate of discarded plastics.

Poster Presentation : **ANAL.P-353**
Analytical Chemistry
Event Hall THU 11:00~13:00

Development of Raman spectroscopic scheme for non-destructive measurement of liver organoid

Sang hoon Cho, Eunjin Jang, Yunjung Kim, Hoeil Chung*

Department of Chemistry, Hanyang University, Korea

In the past, animal testing has been performed on living animals for purpose of assessing the possible negative effectiveness on human. However, it has been issued that problem of ethics like animal abuse and question on the necessity of animal testing when symptom only appears on human. Rather than animal testing, biomedical analysis utilizing an organoid has become an attention-drawing alternative. An organoid is cultivated from human stem cell and has similar cell composition with real organs. Therefore, toxicity test and drug reactions using organoid would be more effective than using other animals. Simultaneously, an analytical tool able to non-destructively analyze a live organoid becomes critically demanding since the destruction of organoid for analysis is not practically allowed for continuation of related toxicological and biomedical research. To meet the demand, Raman spectroscopy based on a wide area illumination (WAI) scheme providing a laser illumination diameter of 1 mm was explored. For the study, normal liver organoids (control group) were cultivated and other organoids were also prepared as non-alcoholic fatty liver (NASH) using culture medium with high fatty acid concentration. Simultaneously, to increase Raman signal of small-size organoids, a cone-shape metal-reflective cavity was prepared and the organoids with culture medium was transferred into the cavity. Then, the WAI scheme covering the whole organoids in the cavity was used to acquire corresponding Raman spectra. Raman spectral features of the control and NASH organoids were compared with each other and their differences were discussed.

Poster Presentation : **ANAL.P-354**
Analytical Chemistry
Event Hall THU 11:00~13:00

Simple determination of Fe_3O_4 concentration in sintered ores by their color images

Woosuk Sohng, Seongsoo Jeong, Hoeil Chung[1,*]

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A sintered ore consists of primarily iron oxides of magnetite (Fe_3O_4) and hematite (Fe_2O_3) with other components such as CaO, SiO_2, and MgO. Since the content of Fe_3O_4 in sintered ore is necessary to determine for stable operation of the process, a titration method based on the redox reaction between Fe^2+ and $K_2Cr_2O_7$ (titrant) has been conventionally adopted; however, it is very slow and cumbersome for sample pretreatment. So, a rapid analytical method for the analysis is highly beneficial. Since the colors of Fe_3O_4 and Fe_2O_3 are black and red, respectively, the colors of sintered ores would be translated into their composition, a driving motivation for this research. With this motivation, color images (pictures) of 200 sintered ore samples with different concentrations of Fe_2O_3 were initially acquired. Then, 2 separate steps were employed to preprocess the image data. First, the difference in RGB values due to the change in brightness of illumination was calibrated (compensated) by using the 3D thin-plate spline warping (TPS-3D) with color-checker. Second, the shades or cracks and features of inorganic oxides except iron oxides were filtered through the image segmentation. Finally, using the 2 step-preprocessed image data, the corresponding Fe_3O_4 concentrations were determined using support vector regression (SVR) and resulting accuracy was comparatively discussed with that based on Raman spectroscopy. Keywords: Sintered ore; Magnetite concentration; Titration; Color image analysis; Support vector regression (SVR)

Poster Presentation : **ANAL.P-355**

Analytical Chemistry

Event Hall THU 11:00~13:00

Back-scattering based axially slanted laser illumination scheme for direct composition analysis of sample housed in a glass container

Haeseong Jeong, Sang Hoon Cho, Hoeil Chung[1,*], Daun Seol[2]

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An axially slanted illumination (ASI) scheme slantingly irradiating laser on the headspace side of a glass container and positioning a detector beneath the container was previously demonstrated to determine gemcitabine concentration (42.9-58.2 wt%) in the gemcitabine injection powder housed in a glass container. Using the ASI scheme, the spectral features of the gemcitabine powder became distinct with only a weak underlying glass background signal. Meanwhile, since the distance between the laser illumination spot and detector location was increased in the ASI scheme, the attenuation of Raman signal was inevitably large. So, it would not adequate to determine concentration of low-level active pharmaceutical ingredient (API) in a housed pharmaceutical sample due to the degraded signal-to-noise ratio. To secure the enhanced signal-to-noise ratio of API peak, a conventional back-scattering (BC) measurement is preferred; however, the strong presence of glass background is problematic. To increase the intensity of API peak with diminished glass background, BC based ASI (BC-ASI) scheme was explored in this study. The BC-ASI scheme tried to incorporate the advantages of both BC and ASI measurements together in one configuration. Use the BC-ASI scheme, pharmaceutical samples (API concentration below 5.0wt%) housed in a glass vial were measured and subsequent accuracy of API concentration determination was compared with those of BC and ASI measurements.

Poster Presentation : **ANAL.P-356**

Analytical Chemistry

Event Hall THU 11:00~13:00

AutoMRM: a targeted proteomics data interpretation tool based on convolutional neural networks and explainable artificial intelligence

<u>Jungkap Park</u>, Jiwon Hong[1], Seunghoon Back[1], Hokeun Kim[1], Sang-Won Lee[1], Sangtae Kim[2,*]

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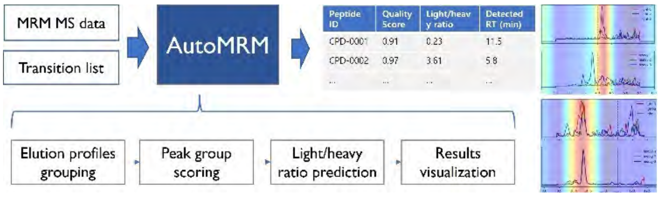
Deep neural networks have led to breakthroughs in discovery proteomics, but their adoption in targeted proteomics has been slow. In clinical proteomics laboratories, researchers spend a significant time on manual peak picking, interference identification, and peak area adjustments to interpret multiple reaction monitoring (MRM) or parallel reaction monitoring (PRM) data. The burden of manual inspection is a major factor limiting transferability, reproducibility, and scalability of targeted proteomics in clinical applications. We present AutoMRM, a targeted proteomics data interpretation tool based on convolutional neural networks (CNN) and explainable artificial intelligence (XAI), designed for clinical mass spectrometry laboratories. When applied to MRM data, AutoMRM shows an accuracy comparable to that of human experts, obviating or significantly reducing the burden of manual inspection. With AutoMRM, an MRM analysis task which used to take over 600 hours by human experts could be completed in less than 5 minutes. We plan to apply the method to the PRM and data-independent acquisition data.



Peptide ID	Quality Score	Light/heavy ratio	Detected RT (min)
CPD-0001	0.91	0.23	11.5
CPD-0002	0.97	3.61	5.8
...	...	...	...

Poster Presentation : **ANAL.P-357**

Analytical Chemistry

Event Hall THU 11:00~13:00

Investigation of multiple strategies for mass spectrometry based proteomic analysis of bronchoalveolar lavage fluid from lung cancer patients

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Mass spectrometry analysis is a prominent technique for clinical proteomics. Several strategies have been developed to advance biomarker identification from liquid biopsies. Bronchoalveolar lavage fluid (BALF) has recently emerged as a promising source of protein biomarkers for lung cancer. However, challenges due to the properties of BALF have limited the sensitivity and specificity of mass spectrometry-based biomarker identification. Therefore, we systemically investigated different approaches, including sample preparation, peptide fractionation, and data acquisition for quantitative proteomic analysis of BALF from lung cancer patients. Herein, we will address the advantages and caveats of each strategy and propose a potential procedure for biomarker identification from clinical samples.

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Poster Presentation : **ANAL.P-358**
Analytical Chemistry
Event Hall THU 11:00~13:00

Structural insights into distinct amyloid aggregation dynamics in water and heavy water

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Department of Chemistry, Korea University, Korea

Amyloidosis is a disease related with oligomer-fibrils formed by self-assembly due to misfolding of amyloid proteins. The self-assembly of amyloid protein is achieved through intermolecular hydrophobic interactions, forming the unbranched beta-sheet structured fibrils. The fibrillation process is not easy to study because it has various fibrillation mechanisms that are affected by various biological factors such as pH, metal ions, and temperature. Examples of such amyloid proteins include α-synuclein, tau protein, and amyloid-β associated with degenerative brain disease. These proteins are intrinsically disordered proteins (IDPs) which do not have a distinct structure, and are proteins with a secondary structure, a random coil. Insulin (INS) is related to a injection localized amyloidosis. Contrary to IDPs, INS is a protein with a distinct secondary to quaternary structure. D2O is generally used as a solvent instead of H2O to observe the protein. However, D2O has different physical properties from H2O due to the isotope effect, which may affect the physical properties of proteins. In the first chapter, we investigated the distinct amyloid fibrillation processes of structured protein, human INS, in H2O and D2O using various spectroscopic tools, including 2D-IR spectroscopy. The following chapter discuss the amyloid fibrillation process of intrinsically disordered proteins, α-synuclein and K18. By employing molecular dynamics simulation, an umbrella sampling method, stability of protofibrils in H2O and D2O can be calculated and compared. Overall, this research aims to understand the H-D isotope effect on protein structures and fibrillation kinetics.

Poster Presentation : **LIFE.P-304**

Life Chemistry

Event Hall FRI 11:00~13:00

Synthesis of photocaged IPTG for producing target proteins in artificial cells

Hyemi Park, Bongjin Moon*

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Artificial cells are an important platform for research on the origins of life, synthetic biology, drug delivery, and gene therapy. However, unlike natural cells, it is difficult to exchange substances actively through the cell membrane since artificial cells have a closed phospholipid bilayer structure. For this reason, metabolites need to be introduced inside artificial cells as inactive precursors when the phospholipid bilayer is formed. The precursors can be transformed into active metabolites by external stimuli such as light irradiation, enzymatic reaction, pH change, or temperature change. Controlling various processes by using light as an external factor in chemical and biological fields has been extensively studied because light can be controlled with high spatiotemporal precision, resulting in minimal sample contamination. In this study, we have synthesized IPTG (isopropyl ß-D-1-thiogalactopyranoside) precursor activated by light irradiation in artificial cells. First, an o-nitrobenzyl (ONB) group was introduced into IPTG as a light-sensitive protecting group and injected into artificial cells. When the artificial cells were irradiated with 300 nm light, it was found that IPTG was released as expected. However, DNA was also damaged by this short wavelength UV light. In order to avoid this problem, we have changed the ONB protecting group to (3,4-methylenedioxy-6-nitrophenyl)-propyloxycarbonyl (MNPPOC) group to make the precursor more active to longer wavelength light.

Poster Presentation : **LIFE.P-305**

Life Chemistry

Event Hall FRI 11:00~13:00

Multi-functional biomineral nanoparticle assembled with tannic acid for tissue engineering applications

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The combined influence of mineral ions, cytokines, and reactive oxygen species (ROS) on regulation of bone regeneration process has been reported. Among them, the excessive ROS level induced by mitochondrial metabolism increases inflammation and infection. Additionally, increase of ROS impairs bone regeneration by hampering osteogenesis.[1] However, conventional biomaterials for bone regeneration only have been developed to endow osteoinductive and osteoconductive properties, but overlooked the control of the overall bone healing microenvironments.[2] Recently, polyphenols have been incorporated within the biomaterials to control microenvironment rich in oxidative stress. Especially, tannic acid, one of the plant derived polyphenol, has a potential in bone regeneration due to its anti-inflammatory, ROS scavenging, and anti-osteoclastogenic activity.[3] In this study, we developed a one-step mineralization method to fabricate multi-functional tannic acid mineral particle (TMP) via self-assembly process using simulated body fluid (SBF) and tannic acid, exploiting rapid metal phenolic network formation. We investigated the ROS scavenging properties and osteogenic effects of TMP using human adipose derived stem cell (hADSC). In addition, anti-inflammatory property of TMP was studied with in vivo mouse peritonitis model. Then, we developed gelatin cryogels incorporating TMP for their application in bone tissue regeneration. We investigated their anti-inflammatory, anti-osteoclastogenesis properties on RAW 264.7 cell and osteogenesis effect on hADSC. In conclusion, our novel multi-functional nanocomposite derived from rapid self-assembly process may suggest effective control tool of microenvironment for bone tissue engineering.

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Poster Presentation : **LIFE.P-306**
Life Chemistry
Event Hall FRI 11:00~13:00

The artificial photosynthetic cellular model for cellular physical activities

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Artificial cellular research has been developing rapidly, and some researchers have already shown several different cellular cascade bioreactions using their artificial cellular models. However, researchers have not thoroughly researched cellular physical activities using artificial cellular models yet. Most cellular physical activities require diverse interactions between cytoskeletal proteins and plasma membranes. However, creating these interactions in artificial models with a bottom-up approach is exceptionally challenging. Due to the difficulties, most scientists mimic the cellular systems in vitro instead, but it is limited to understanding the interactions and dynamic networks between the compartments in cells. Also, vesicle experiments have several difficulties inhibiting the chemicals trespassing between membranes for bioactivity mimicry without any additional transmembrane proteins. Therefore, we designed and built an artificial cellular model that overcomes both in vitro and vesicle experiments research limitations that explain the several different networks and interactions between differently conditioned membranes and self-polymerizing cytoskeletal proteins (F-actin). Our research model, the giant unilamellar vesicles (GUVs), contained ATP generating artificial photosynthetic organelles. We triggered and controlled the actin polymerization by light, which controls the ATP production of the artificial photosynthetic organelles. As the cytoskeletal filaments grew in the GUVs, they showed different morphologies by the diversity of GUV membranes following the characteristics of cellular membranes: ordered/disordered phases from saturated/unsaturated, charged/zwitterionic, or cholesterol-free/cholesterol-containing phospholipids. We divided the morphologies into three conditions, no interactions, interactions, and the creation of an inner crust. Therefore, our model could be the best model with a minimal limitation for determining the cytoskeletal-membrane interaction, which could mimic physical cellular activities.

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Poster Presentation : **LIFE.P-307**

Life Chemistry

Event Hall FRI 11:00~13:00

A FRET-based probe to simultaneously detect both O-GlcNAcase and phosphatase

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In higher eukaryotes, thousands of cytoplasmic and nuclear proteins are post-translationally modified with a single monosaccharide, N-acetylglucosamine (GlcNAc), that is O-linked to serine (Ser) or threonine (Thr) side chains (O-GlcNAc). The O-GlcNAc glycosylation of proteins is a highly dynamic process that frequently interplays with protein phosphorylation. Both modifications conducted by O-GlcNAcase and phosphatases are involved in various cellular events. Abnormal levels of these modification are closely correlated with diverse diseases such as diabetes, cancer, and neurodegenerative disorders. Thus, it is highly important to detect these enzymes in cells. In this study, we designed, prepared and evaluated the usefulness of a FRET-based fluorescent probe, which can be utilized to detect O-GlcNAcase and phosphatases in live cells.

Poster Presentation : **LIFE.P-308**

Life Chemistry

Event Hall FRI 11:00~13:00

Exploration of Sequence-based Design for α/β/γ-Peptide Foldamer Mimicking BH3 Helical Domain

Young-Hee Shin[*], SangHun Woo, Jung Jihoo

Department of Chemical Engineering & Biotechnology, Korea Polytechnic University, Korea

A sequence-based design by incorporation of α-, β- and γ-amino acid residues engenders a stable helical secondary structure that mimics an α-helix. Previous studies have shown that an αγααβα hexad motif leads to a helix with β and γ residues aligned along one side and the remainder of the surface dominated by α residues. These helices are much more prone to folding in aqueous solvents than are conventional peptides of comparable length. In this study, we applied this α/β/γ-peptide foldamer design strategy to mimicry of BH3 helical domain, Bim, as a pioneering study for functional α/β/γ-peptides development. The Bim-based α/β/γ-peptides in an αγααβα-hexad repeat with five helical turns inhibited the interaction between Bak and Bcl-xL with excellent resistance against proteolytic digestion. Our study suggests that α/β/γ-foldamer can be developed as an alternative general platform for the sequence-based peptide design researches especially with prominent resistance to enzymatic digestion.

Poster Presentation : **LIFE.P-309**

Life Chemistry

Event Hall FRI 11:00~13:00

CAIX-Targeting Controllable Self-Assembly of Peptide Amphiphile with Membrane Interaction Inducing Cellular Apoptosis

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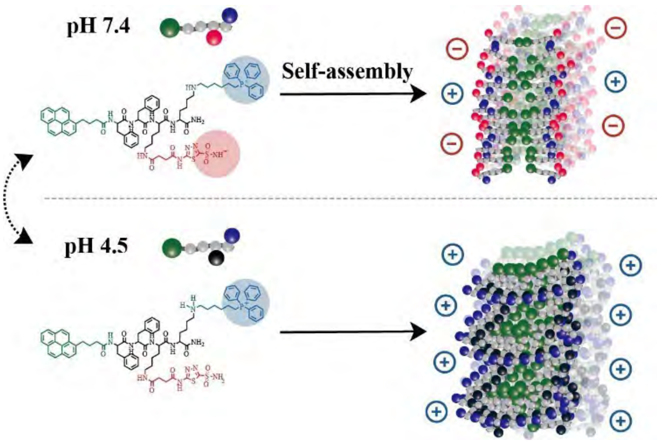
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

The controllable peptide self-assembly has been emerged as novel strategy for modulating cellular behavior. Since cellular milieu is highly dynamic, cellular fate can be precisely controlled when proper spatiotemporal control is achieved. In order to achieve spatiotemporal control inside cells, enzyme instructed self-assembly has been widely used. However, this strategy usually exhibits a minimal impact on the cellular fate. Recently, studies have been reported to directly modulate cellular fate by disrupting lipophilic membrane using self-assembly with high positively charged bioactive epitope. Herein, we designed Pep-AT, functionalized by acetazolamide and triphenylphosphonium (TPP), in which self-assembly behavior can be tuned depending on pH. At pH 7.4, a large aggregate with negative surface charge is formed due to deprotonation of acetazolamide. However, a highly ordered self-assembly structure with positive surface charge is formed at pH 4.5 with protonation of acetazolamide. At the cellular level, Pep-AT can target CAIX selectively overexpressed cancerous membrane, and trapped into lysosome via CAIX-mediated endocytosis in spatiotemporal manner. At only lysosome environment, Pep-AT can interact and disrupt the membrane due to presentation of high positive charge, and induce cellular apoptosis. This study demonstrates controllable self-assembly system at cellular level in combination with enhancement for the interaction with lipophilic membrane. Thus, this system presents the possibility of further application into cancer therapy by modulating cellular behavior directly.


pH 7.4
Self-assembly
pH 4.5

Poster Presentation : **LIFE.P-310**

Life Chemistry

Event Hall FRI 11:00~13:00

Supramolecular hyper-branch polymerization using Host-guest interaction

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Among supramolecular chemistry, host-guest interactions describe two molecules that interact based on non-covalent bonds. Non-covalent bonds are weaker than covalent bonds but are used to make large molecules such as proteins and nucleic acids that are important for biochemical processes. In this work, we designed AOCB[6]-PY, in which host and guest molecules are linked, to become a tunable hyperbranched polymer through host-guest interactions. Cucurbit [6] uril (CB [6]) is a non-toxic host material that does not fully interact with the guest material pyridine at room temperature, but at high temperatures the activity of the host and guest molecules increases, forming a hyperbranched polymer. Therefore, we developed reusable hyperbranched polymers using temperature-dependent host-guest interactions to achieve antimicrobial polymer coatings.

Poster Presentation : **LIFE.P-311**

Life Chemistry

Event Hall FRI 11:00~13:00

The Use of Oxford Nanpore MinION Sequencing for Detection of Enzyme Targeting Sites on DNA

Myungheon Yu, Kyubong Jo[1,*]

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[1]*Department of Chemistry, Sogang University, Korea*

The visualization of DNA molecules using fluorescent dyes or fluorescent protein tagged DNA binding proteins (FP-DBP) has been used to observe specific sites where enzymes act on DNA. However, it is difficult to determine the more accurate sites where the enzyme acts and distinguish specific binding sites from unspecific binding sites. In this research, we introduced the Oxford Nanopore MinION sequencing to detect enzyme targeting sites on DNA as a new approach. Oxford Nanopore sequencing is cost-effective, portable, and time-saving compared to other Next-Generation Sequencing (NGS). DNA fragments containing nicking enzyme targeting sites were isolated from the rest through a precipitation and each was sequenced with MinION sequencer. The nicking enzyme targeting sites were shown more precisely in Integrative Genomics Viewer (IGV) in comparison with DNA visualization. Also, it was possible to identify which strand of the dsDNA had the nicking site, since the direction of DNA polymerase could be recognized. This approach could be more simplified by omitting precipitation when DNA binding protein targeting sites were detected. DNA fragments unbound to proteins were only sequenced as proteins bound to dsDNA blocked the entrances of the nanopores. In summary, Oxford nanopore sequencing could be a powerful tool for detection of enzyme targeting sites on DNA.

Poster Presentation : **LIFE.P-312**
Life Chemistry
Event Hall FRI 11:00~13:00

NMR dynamics study of the contribution of the α4 helix of human TALE TF, PBX4 to DNA binding

Youyeon Go, Joon-Hwa Lee*

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Three amino acid loop extension (TALE) homeodomain proteins are a proline-tyrosine-proline (PYP)motif and are located between the first and second helix of the HD of a highly conserved DNA binding domain of approximately 60 amino acids called the homeodomain. The three amino acid loop extension (TALE) homeodomain proteins are a family of transcription factors including the mammalian PBX, MEIS and PREP proteins. PBX4 protein belongs to the TALE family characterized by a Three-Amino-Acid Loop Extension within the homeodomain of these proteins. It activates the ephA8 transcription and it unconsciouss, the Pbx transcription factor protein controls the movement control of eye. Unlike other Tale homeodomain proteins, PBX4 proteins have a-helix4. We studied the wild type PBX4(PBX4-EX)−pbxDNA and mutant PBX4(PBX4-HD)−pbxDNA interactions using imino proton and heteronuclear singlequantum correlation (HSQC) titrations. In this study, we performed NMR experiments on complexes of several wild type of PBX4 with the wt-pbxDNA duplex at various protein-to-DNA (P/N) molar ratios. We also determined the thermodynamic parameters for DNA binding of PBX4-EX and PBX4-HD using Isothermal titration calorimetry (ITC). This study provides information about the conformational differences in DNA recognition of α-helix4 of PBX4.

Poster Presentation : **LIFE.P-313**

Life Chemistry

Event Hall FRI 11:00~13:00

Development of Amidobezimidazole derivatives as STING agonists

Hye Lim Lee, Sanghee Lee*

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The stimulator of interferon genes (STING) is an important regulator of anti-viral response and innate immune system. The aberrant appearance of exogenous or endogenous DNA or infection of DNA pathogens triggers the activation of the Cyclic GMP-AMP synthase(cGAS)-STING signaling pathway. Activation of STING induces the production of type 1 interferon which stimulating innate immune response in tumor microenvironment, priming T cells, and infiltrating T cell into tumor, thereby promotes anti-tumor immunity by alteration of tumor Immunophenotype. Therefore, the strategy for activating STING has been considered as a potential therapeutic target for next generation cancer immunotherapy. Based on high-throughput screening, we discovered a new chemical entities that effectively activated STING pathway and innate immune response.

Poster Presentation : **LIFE.P-314**

Life Chemistry

Event Hall FRI 11:00~13:00

Kinetic Study of Multivalent Protein-Protein Interactions upon Valency

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Multivalent interaction is an extensively used strategy in the research area as well as in nature because it enables to achieve high selectivity and affinity. But research to prove the detailed mechanism such as kinetic properties of multivalent interactions are very scarce. To find kinetic principles that underlie multivalent protein-protein interactions, here we established a fully protein-based model system having programmed valency. We investigated the changes of kon and koff values through the valency change by surface plasmon resonance (SPR). Carefully selected protein binding pairs separately fused to oligomeric backbones, and one side of the pair was attached to the SPR chip in an orientation-controlled manner. Counter-part of the pair was flowed over the surface and examined upon varied valencies. We attained kon and koff values by Langmuir binding model from 1:1 to 4:4. We demonstrated that the multivalency gave more effect on koff than on kon, resulting in enhancement of avidity. Additionally, we observed smeared bands in polyacrylamide gel electrophoresis (PAGE) analysis, when koff value of high valence isn’t low enough. Variation of kon, however, depended on the type of the ligands rather than the valency. This research is the first example of investigating the multivalent interaction of proteins. It would be the stepping stone for understanding the kinetic property of multivalent protein-protein interaction.

Poster Presentation : **LIFE.P-315**

Life Chemistry

Event Hall FRI 11:00~13:00

Development of MC1568 derivatives exhibiting therapeutic potential to prevent depression via HDAC11 inhibition in microglia

Jeehee Lee, Sanghee Lee*

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Histone deacetylases (HDACs) are key epigenetic regulators, and the 18 different HDAC isoforms are classified into four subtypes. Despite the various roles of each HDAC isoform, the lack of selective HDAC inhibitors has limited the elucidation of their individual roles. Based on the modification of MC1568, we developed a HDAC inhibitor, 5, that specifically inhibits HDAC6, 8, and 11. Interestingly, HDAC inhibitor 5 initiated autophagy, inhibited the production of nitric oxide, and suppressed lipopolysaccharide-induced microglial activation by regulating the deacetylase function of HDAC11. Furthermore, we demonstrated that 5 significantly alleviates depression-like behavior in mice. The role of HDAC11 in microglia is not fully understood, even though it is highly expressed in the brain. Therefore, our discovery of HDAC11 inhibitor revealed the role of HDAC11 in autophagy and reactive nitrogen species balance in microglia.

Poster Presentation : **LIFE.P-316**

Life Chemistry

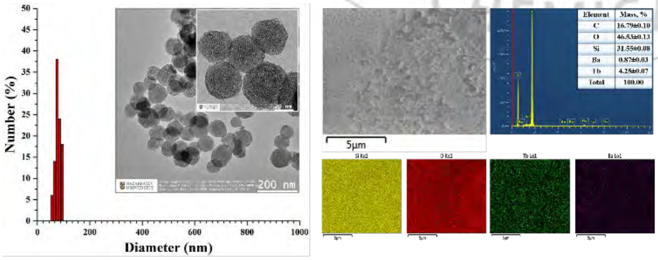
Event Hall FRI 11:00~13:00

Ba and Tb Co-doped SiO2 Nanoparticle for Theragnostic Application

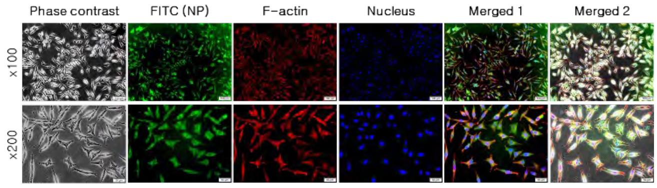
Moon Sung Kang, **Hee Jeong Jang, Seokhyun Lee, Dong-Wook Han***

Department of Cogno-Mechatronics Engineering, Pusan National University, Korea

In recent years, there is a great interest in the development of multifunctional nanostructures suitable for theranostic applications. The main goal of this preliminary report is to construct metal-doped SiO2-based nanoparticles (NPs) that can be potentially useful for bioimaging and drug delivery purposes. It was found that Ba and Tb co-doped SiO2 NPs have a spherical morphology, narrow size distribution (70-80 nm), and high specific surface area (573.9 m2/g). We showed that Ba ions incorporation makes these NPs efficient for X-ray attenuation in computed tomography CT, while the Tb ions endow them with excellent photoluminescent properties. In particular, Ba-Tb-SiO2 NPs demonstrated a promising X-ray attenuation value of ~ 30.8 HU/mM. The luminescent properties of prepared NPs were associated with characteristic Tb (III) 5D4-7Fj (j = 3, 4, 5, and 6) transitions with the absolute quantum yield of ~ 12.2 %. It is suggested that the proposed method can be extended for the incorporation of other ions to develop new theranostic nanoprobes.



Element	Mass, %
C	16.79±0.10
O	46.53±0.13
Si	31.55±0.08
Ba	0.87±0.03
Tb	4.25±0.07
Total	100.00



Poster Presentation : **LIFE.P-317**

Life Chemistry

Event Hall FRI 11:00~13:00

MiLearn^{TM}: An Artificial Intelligence Platform for Drug Discovery and Development- Validation of Artificial Intelligence Models for Target-based Drug Discovery -

Seungju Lee, <u>Yuna Ha</u>, Eun Sub Song, Minwoo Han*, Jee-Young Lee[1,*]

Molecular Design Team, SBDD, New Drug Development Center, K-Medi hub, Korea
[1]*Structure-based Drug Discovery (SBDD) Laboratory, New Drug Development Center, K-Medi hub, Korea*

MiLearn^{TM} is an artificial intelligence platform for drug discovery and development. Several AI models are included in this platform, and two models (DeepPro, AutoG) for target-based drug discovery are intorduced to this poster. DeepPro is a model for predicting the binding affinity of drugs based on the 3D data of target-drug binding structure, and AutoG is a deep learning model that uses molecular dynamics simulation to classify whether GPCR agonist or antagonist. In this study, performance of the AI models were verified through the discovery of Kinase and GPCR hits, and upgrade strategy of models were suggested.

Poster Presentation : **LIFE.P-318**

Life Chemistry

Event Hall FRI 11:00~13:00

Pore Formation on Artificial cell Membrane using Melittin

Kwanwoo Shin*, SeonMin Jeon

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The nucleus is one of the most important organs in the cell. It protects genetic information and regulates gene expression and the activity of cells. DNA replication and mRNA transcription occur inside the nucleus. And synthesized mRNA is sent to the cytoplasm through the nuclear pore. If we combine the system that synthesizes DNA or mRNA inside the artificial cell and sends mRNA out through the pore, it could be another model of the artificial nucleus. In this study, we aimed to make pores on artificial cell membranes using a peptide called Melittin. Melittin is a major pain-producing substance of bee venom that causes cell lysis and antimicrobial activity. Melittin has a high degree of amphiphilicity and a net positive charge. When Melittin binds to the bilayer horizontally due to its hydrophobic residue, melittin generates stress to the membrane and forms a pore. By this study, we expected that pores on the phospholipid membrane made by Melittin can be the model of the nuclear pore.

Poster Presentation : **LIFE.P-319**

Life Chemistry

Event Hall FRI 11:00~13:00

Design and fabrication of pump-less microfluidic PCR devices for point-of-care testing

Eunjin Huh, Hyuckjin Lee, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Polymerase Chain Reaction (PCR) is a well-known technique for replicating and amplifying specific DNA sequences and is used in many fields including disease diagnosis, forensic analysis, and DNA cloning. Researchers have developed microfluidic devices to reduce analysis time, but most of the devices rely on bulky pumps or motors. Furthermore, most devices have fixed PCR cycles, making it difficult for users to change the temperature or cycle. We designed gravity-driven rotary PCR devices to optimize both advantages and disadvantages. The device can be used with the two-temperature, shuttling PCR protocol: one for denaturation and another for combined annealing and extension. A preliminary heating test showed that each temperature region provided an appropriate environment for each PCR step. The device has a stepper motor that rotates the space in which the sample is mounted and repeatedly moves the fluid. A microcontroller controls the heater and motor so that the fluid moves by gravity without a pump. Many chips have been used to solve the evaporation and number of samples problems, and the design and each test result will be presented in this presentation.

Poster Presentation : **LIFE.P-320**

Life Chemistry

Event Hall FRI 11:00~13:00

A new class of N-terminal cysteine assay: Characterization of De novo formation of citrate-based fluorophores for analysis of proteins

Yun Jung Choi, Jinyoung Pac[1], Yan Lee[*]

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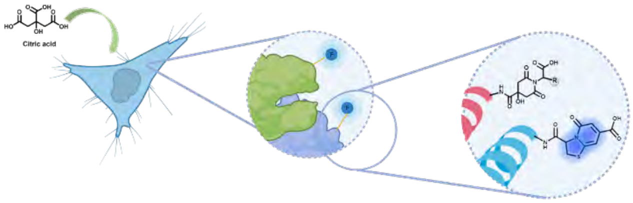
[1]*Seoul National University, Korea*

Fluorescence detection has become widely used tools in various fields such as biochemistry. Since it has superior selectivity and sensitivity to absorbance detection. In biochemistry, fluorescence technique can be used as microarrays, fluorescence spectroscopy and fluorescence imaging. Especially, fluorescence microscopy has become promising technique for monitoring various cell organelles and tissues to the fore. For example, chemical fluorophores such as fluorescein, rhodamine, BODIPYs, and cyanine (Cy5) are still in use wildly. However, chemical fluorophores likely to have cellular toxicity. On the other hand, biological fluorophore, such as GFP, is non-toxic but too bulky.Therefore, there is a need to develop a new fluorophore having low toxicity, high quantum yield, and small size for high penetration. We tried to develop the fluorophore which has the advantages of chemical fluorophores and biological fluorophores. As a proof of concept, we investigated the De Novo formation of blue fluorophore (TPA), from citric acid and cysteine. Use of an amide coupling reagent (PyBOP) greatly facilitates the fluorophore formation on peptides and proteins with N-terminal cysteine.Through series of experiments using amino acids, peptides, and proteins, we confirmed that only Cys with free amine and thiol groups can produce the blue fluorescence in the condition. Moreover, intracellular or extracellular peptides and proteins with N-terminal Cys were fluorescently labelled in a spatially-specific manner by the DNFC method. The DNFC method, which exhibits characteristic distributions of fluorescently labelled proteins in biosamples. The DNFC staining is able to provide a new potential protocol for future cell imaging, histology and diagnosis.


Citric acid

Poster Presentation : **LIFE.P-321**
Life Chemistry
Event Hall FRI 11:00~13:00

SARS-CoV-2 Model: Controllable Array of Recombinant Spike Protein on Synthetic Liposome

Hyun Park, Huong Thanh Nguyen, Kwanwoo Shin[1,*]

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With the outbreak of COVID-19 pandemic caused by the severe acute respiratory syndrome coronavirus 2(SARS-CoV-2), the study for this virus is now emerging as the most important issue to be addressed. In the research of coronavirus, understanding the whole mechanism toward human cells is very complicated and multilayered, due to their complex components and assembly of the viral particles. Although all the components contribute to their functions, there are some critical components for coronavirus: closed lipid bilayer membrane for maintenance of the structure, viral antigens such as Spike (S) protein for viral entry. Therefore, we attempted to make a liposomal virus model focusing on the qualitative and quantitative features of the virus that could understand the biological behavior of the coronavirus. Here, we constructed a SARS-CoV-2 model by conjugating polyhistidine-tagged (His-tagged) S protein on the surface of Ni-NTA functionalized liposomes in controlled quantity and oriented direction. The His-tagged protein was strongly attached to the surface of the liposome, and their activity as a virus model has been validated with antigen diagnosis kit. The ratio of antigen per liposome was also determined precisely by phosphorous assay and immunoassay. With this simplified structure from the virus, this model is expected to be used for various research fields such as diagnosis kit validation, mechanism of viral entry, and development of new vaccine candidates with reduced risk of infection.

Poster Presentation : **LIFE.P-322**

Life Chemistry

Event Hall FRI 11:00~13:00

Cannabidiol Protects Primary Hippocampal Neurons against Hydrogen Peroxide

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(–)-Cannabidiol (CBD), a major non-psychotropic phytocannabinoid derived from the *Cannabis* genus, has shown great therapeutic potential on neurological diseases, but its biochemical mechanism remains elusive. In-vitro studies with primary hippocampal neurons have been conducted to investigate the neuroprotective effect of CBD against hydrogen peroxide (H_2O_2) as well as the neurotoxicity profile of CBD. While CBD exhibits 9.85 μM of LD_{50} with detachment-induced apoptosis in the in-vitro setting, it noticeably protects the neurons against H_2O_2 (10 μM) in a concentration-dependent manner. The neuroprotection ratio of CBD against H_2O_2 was 2.40 with 5 μM of CBD (viability increase from 24% to 57%). In addition, CBD rescues the impairments of neuronal morphology induced by oxidative stress.

Poster Presentation : **LIFE.P-323**

Life Chemistry

Event Hall FRI 11:00~13:00

NMR study of consensus DNA recognition of transcription factor HOXA1

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In humans, the Hox genes are distributed into four linkage groups, HOXA, HOXB, HOXC, and HOXD, which locate on chromosomes 7, 17, 12, and 2, respectively. HOXA1 is thought to be involved in the placement of hindbrain segments in the proper location along the anterior-posterior axis during development. Homeodomain (HD) protein has 60 amino acids which are highly conserved in α1 and α3 helices. The N-terminal arm (L1) and loop regions (L2 and L3) between the helices are also well conserved. Interestingly, the second and third residues in L1 loop are conserved as the positive charged residues, Lys(K) or Arg(R), among almost all HOX proteins. However, the HOXA1 has residues Asn(N) and Ala(A) in position 2 and 3 instead of K and R. In order to understand molecular mechanism of DNA recognition of HOXA1, we have performed NMR experiments on the homeodomain of HOXA1 (HOXA1-HD) complexed with 10-bp consensus DNA (included TAAT) and 10-bp mutant DNA duplexes (included TGAT, TCAT and TTAT), at a variety of DNA-protein molar ratios. In addition, to clarify the role of residues 2 and 3 in Loop 1, we prepared HOXA1-KR mutant in which residues N2 and A3 are replaced by K2 and R3, respectively, and compared its structural feature in a complex with DNA with those of wild-type HOXA1-HD. We also determined the thermodynamic parameters for each DNA binding of WT HOXA1-HD and HOXA1-KR mutant using Isothermal titration calorimetry (ITC). Our study provides an insight into the role of residues N2 and A3 during target DNA recognition of HOXA1.

Poster Presentation : **LIFE.P-324**

Life Chemistry

Event Hall FRI 11:00~13:00

NMR study on MEIS1, a human transcription factor that binds to consensus DNA

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Transcription factors are proteins that bind specific sites or elements in regulatory regions of DNA, known as promoters or enhancers, where they control the transcription or expression of target genes. MEIS1 (myeloid ecotropic viral insertion site 1) is a viral integration site in murine myeloid leukemia cells. This gene encodes a homeobox protein belonging to the TALE ('three amino acid loop extension') family of homeodomain-containing proteins. TALE proteins are distinguished by the presence of three extra amino acids in the loop binding the first to the second alpha helix of the homeodomain. The highly conserved DNA binding TALE proteins define the family and is responsible for specific recognition of a common sequence motif, [5'- TGACA- 3']. Further DNA binding specificity within TALE family members is determined by adjacent DNA sequences and through the binding of additional transcriptional partners. In order to characterize the molecular recognition of DNA by MEIS1, we performed NMR experiments on MEIS1 complexed with 10-bp DNA duplex, d(AGCTGACAGC)/ d(GCTGTCAGCT), (wt-msDNA) and its mutants using NMR. We also studied the binding features of MEIS1 for both wild type and mutant DNAs characterized its target DNA recognition.

Poster Presentation : **LIFE.P-325**
Life Chemistry
Event Hall FRI 11:00~13:00

Antifungal effect of nano-emulsions encapsulated with essential oils

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Recently, natural essential oils have been actively conducted as an eco-friend alternative substance for preservation and antifungal, due to their non-toxicity. In this study, the antifungal effects of the nano-emulsions in an aqueous phase were investigated to reduce the food quality degradation by fungi or microorganisms. The nano-emulsions were prepared in an aqueous solution with essential oils, D-Limonene, Lemongrass, and Oregano. The aqueous phase nano-emusion were mixed with 4 wt% essential oil, 0.5 wt% emulsifier, and distilled water. The mixed solution was treated with a high-speed rotator at 10,000 rpm for 5 minutes and then homogenized twice at 20,000 psi using an ultra-high pressure homogenizer. The particle properties of prepared emulsions, such as Zeta potential and particle size, were measured by a particle size analyzer. The size distribution was 150 ~300 nm and Zeta potential was - 30 mV ~ - 35 mV. In addition, the encapsulated efficiency of essential oil was analyzed by Beer-Lambert law. The antifungal effect of prepared emulsions was investigated in Penicilliun expansum (KACC 40814), Botrytis cinerea (KACC 40754) in a solid badge. The concentration of fungi was diluted by a fourth, and 30 ul was spread on the surface of solid badges. 2 ~ 8 ml of emulsion was treated to the cellulose fiber by a step of 2 ml. The germination of fungi was measured by a step of 24 hours. The antifungal effect of emulsions clearly was observed in comparison with that of a non-treated cellulose fiber.

Poster Presentation : **LIFE.P-326**

Life Chemistry

Event Hall FRI 11:00~13:00

NMR Study of Transcription Factor protein DLX3 and TF-DNA complex

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Transcriptional factors(TFs) are protein that promotes or inhibits gene expression by binding to a specific site of DNA called a response element near the eukaryotic cell gene. The DNA-binding domain(DBD) of the transcription factor binds to the DNA of specific sequence called enhancer. Among them, DLX3(Drosophila distal-less homeobox 3) gene is expressed throughout development in a series of structures derived from epithelial-mesenchymal interaction such as the teeth, hair follicles, and limb buds. DLX3 mutations have been found to be responsible for Tricho-Dento-Osseous(TDO) syndrome. The highly conserved DLX3 is responsible for specific recognition of a common sequence motif, [5'- TAATTG-3']. We find the molecular mechanisms of specific DNA recognition in DLX3 through HSQC titration of [5'-TAATTG-3’]-DNA. The exchange rate constants of the imino protons for the [5'-TAATTG-3’]-DNA, and TF-DNA complex were measured by using water magnetization experiment.

Poster Presentation : **LIFE.P-327**

Life Chemistry

Event Hall FRI 11:00~13:00

Synthesis of a DNA-Encoded Library of Pyrrolo[2,3-d]pyrimidines

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[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Developing DNA-encoded libraries of privileged scaffolds, such as pyrrolopyrimidines, is of great interest in drug discovery and chemical biology as a powerful tool to rapidly and inexpensively discover potent drug candidates. However, it is often challenging to construct such DNA-encoded libraries because many reaction conditions are not compatible with DNA. Here, we describe the development of a convenient solid-phase synthetic strategy that overcomes the current limitations and allows the efficient synthesis of a DNA-encoded combinatorial library of structurally diverse tetra-substituted pyrrolo[2,3-d]pyrimidines.

Poster Presentation : **LIFE.P-328**

Life Chemistry

Event Hall FRI 11:00~13:00

Investigation of Microorganisms Inactivation Under Extreme High Pressure

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High pressure, a wide range of temperature, pH, salinity, light intensity, and low oxygen concentration affected the microorganisms and encouraged the microorganisms to adapt to the extreme environment. As one of the crucial aspects of the living conditions of microorganism, high pressure has the potential to induce the inactivation of microorganisms through the destruction of proteins and membranes.[1] Escherichia coli (E. Coli) and Bacillus subtilis (B. subtilis) are widespread bacteria, representing gram-negative and gram-positive bacteria. In this study, E. coli and B. subtilis were subjected to high maximum pressure of 0.5 GPa for 10 minutes inside a diamond anvil cell system to observe the phenomena mentioned above. Survived bacteria were examined by platting methods, assumed that survived and healthy bacteria could form the new colonies. When the bacteria were treated with 50 MPa pressure, the number of E. coli and B. subtilis that could survive was the same as untreated bacteria. However, after the pressure increased up to 0.5 GPa, both E. coli and B. subtilis ultimately died. On the other hand, high pressure has potential to change the morphology of bacteria and increase the bacteria doubling time based on the preliminary result. Therefore, a further study is needed to understand those two interesting points which may related to the gene of the bacteria.Keywords: High pressure, bacteria, E. coli, B. subtilis, diamond anvil cellReference:1.Ulmer, H. M.; Gänzle, M. G.; Vogel, R. F., Effects of high pressure on survival and metabolic activity of Lactobacillus plantarum TMW1.460. Applied and environmental microbiology 2000, 66 (9), 3966-3973.

Poster Presentation : **LIFE.P-329**

Life Chemistry

Event Hall FRI 11:00~13:00

Fluorescence Imaging of Cells and Tissues using Fluorophores Generated in the Biosystem

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Optical tissue imaging has gained much attention as techniques which enables to analyze and visualize biological samples. Fluorophore tagged molecules are utilized to label the target of interest and as the gold standard in bioimaging. However, most fluorophores are synthesized prior to the introduction to the biological samples, and false-positive signals due to non-specific binding of the fluorophores often limit the accurate evaluation of the biological information. Thus, if the fluorophores can be generated from non-fluorescent precursors on a specific target in biosamples, it would greatly reduce the false-positive signals in bioimaging and provide more accurate information of biomolecular distribution in the sample. In this study, we applied DNFC, de novo formation of formation of citrate-based fluorophore, to label cells and tissues. Through DNFC, non-fluorogenic citrate forms bright fluorophores on the N-termini of proteins under mild reaction conditions. This turn-on response of fluorescence provides the molecular distribution of biomolecules with advanced analytic accuracy compared to conventional fluorescent labeling techniques which introduce a pre-synthesized fluorophore to the cells and tissues. Based on this fluorogenic reaction, we could visualize various biological samples such as organs and lesions in human tissues with enhanced emission intensity. We believe that DNFC-based optical tissue imaging could be a supporting method for conventional tissue staining techniques in histology and histopathology by providing additional information with better accuracy.

Poster Presentation : **LIFE.P-330**

Life Chemistry

Event Hall FRI 11:00~13:00

Self-assembly Study of Collagen Fibrils from Type I Collagen Monomer under Electric Fields and Its Application

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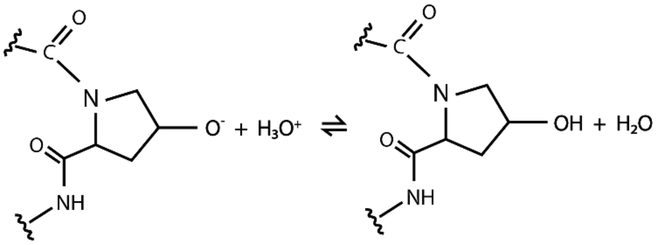
Department of Chemistry & Institute of Biological Interfaces, Sogang University, Korea

Collagen is one of the prominent scaffolding components of the extracellular matrix that can turn into collagen fibers through self-assembly mechanisms. Understanding that various factors can influence collagen assembly, we studied the effect of electric field exposure and visualized collagen fibrils' fibrillogenesis process under the confocal microscope. Collagen monomers started to aggregate within 10 seconds after applying an AC of 10 Hz-1V, and collagen fibrils with a 28 to 70 nm diameter appeared within 9 minutes. Further, we designed an experiment to form collagen fibers at a targeted region by encapsulating collagen molecules in nano-sized liposomes (Lip-Col) and have confirmed that the fibrils were successfully formed. We infer that the electric field could trigger the electrical interaction between hydronium ion and the hydroxyl group of hydroxyproline in the peptide chains of collagen, resulting in the change of the surface charge of the collagen and pH solution. In vitro, Lip-Cols can interact with the cellular membrane of human dermal fibroblast and form collagen networks in extracellular matrix space. Our findings can potentially be utilized as a material coating method and a drug delivery system for anti-aging or wound healing agents.



Poster Presentation : **LIFE.P-331**
Life Chemistry
Event Hall FRI 11:00~13:00

NMR dynamics Study of miR390a Precursor

Ho-seong Jin, Joon-Hwa Lee[1,*]

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[1]*Department of Chemistry, Gyeongsang National University, Korea*

miRNAs originate from primary transcripts containing self-complementary hairpin structures that are initially processed to form 21~22-nt miR/miR* duplexes. In plants, primary transcripts with miRNA foldbacks (pri-miRNAs) are processed by the RNase-III like enzyme DICER-LIKE1 to generate miR/miR* duplex. The levels of mature miR390 influence the leaf number prior to flowering in the life cycle of plants. To understand the molecular mechanism of biogenesis of primary miR390a (pri-miR390a) to mature miR390, a NMR hydrogen exchange study was performed using model RNAs mimicking the cleavage site of wild-type and bulge-stabilizing mutant pri-miR390a constructs. Our results suggest that the stabilities of the two base-pairs at the cleavage site are essential for formation of the active conformation and for efficient processing of pri-miR390a.

Poster Presentation : **LIFE.P-332**

Life Chemistry

Event Hall FRI 11:00~13:00

Preparation of a Multiple-Targeting NIR-Based Fluorogenic Probe and Its Application for Selective Cancer Cell Imaging

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Department of Chemistry, Yonsei University, Korea

To improve cancer selectivity of imaging agents, we synthesized the triple-targeting, near-infrared (NIR) based fluorogenic probe, Oct-FK(PBA)-NIR. The new probe consists of (1) octreotide as a synthetic ligand of somatostatin receptors, (2) a H2O2-responsive phenylboronic acid, (3) a dipeptide substrate for cathepsin B, and (4) a NIR fluorophore. The results of cell studies show that the probe can be used for selective imaging of cancer cells in the NIR range without interference with normal cells.

Poster Presentation : **LIFE.P-333**

Life Chemistry

Event Hall FRI 11:00~13:00

Selective cancer cell death using metabolic glycan labeling technique

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Yonsei University, Korea

[1]*Department of Chemistry, Yonsei University, Korea*

Metabolic incorporation of glycan precursors possessing clickable units into cellular glycans has become a useful method to probe glycosylation in cells, tissues and organisms. One major challenge in applying this method is to develop approaches that enable incorporation of glycans into specific types of cells. As part of this effort, we developed a method for inducing cancer cell death, which relies on the use of a H2O2-responsive glycan metabolic precursor in conjunction with photodynamic therapy (PDT). When cancer cells were incubated with the H2O2-responsive glycan metabolic precursor, it was incorporated into cell-surface glycans. The cell-surface azide-possessing glycans were then labelled with photosensitizer (PS) via click chemistry. The cell study showed that singlet oxygen produced during PDT promotes apoptosis of cancer cells via caspase activation.

Poster Presentation : **LIFE.P-334**

Life Chemistry

Event Hall FRI 11:00~13:00

Dexamethasone-loaded poly(lactic-*co*-glycolic acid) (PLGA) microparticles with strong calcium-binding affinity for alleviation of surgery-induced osteitis in sinonasal cavity

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Many chronic rhinosinusitis (CRS) patients with limited response to medical therapy often undergo endoscopic sinus surgery (ESS). However, inevitable mucosal detachment and bony exposure during the surgery initiate the development of osteitis, which eventually leads to the recurrence of CRS. Although oral or intranasal administration of corticosteroid is commonly used to treat ESS-induced osteitis, such methods have critical limitations and may provoke serious side effects. Therefore, localized corticosteroid delivery at effective concentration on the wounded area is very crucial. To tackle these problems, we designed dexamethasone (Dex)-loaded poly(lactic-*co*-glycolic acid) (PLGA) microparticles with bone-specific binding affinity, releasing encapsulated Dex in a sustained manner on the exposed nasal bone after ESS. Along with biocompatible and biodegradable PLGA core, previously reported poly(butyl methacrylate-*co*-methacryloyloxyethyl phosphate) (PBMP), containing both calcium-binding phosphomonoester groups and PLGA-binding butyl groups, was coated on the particle surface to introduce strong calcium-binding property. Interestingly, PBMP-coated PLGA particles encapsulating Dex (Dex-PLGA/PBMP) revealed over 5-times higher hydroxyapatite (HA) binding affinity compared to the non-coated PLGA particles without changing the morphology and encapsulation efficiency. Intranasally administered Dex-PLGA/PBMP in the mouse model with mechanically injured nasal mucosa showed the inhibition of new woven bone formation and promotion of wound healing. Furthermore, significantly lower osteocalcin activity, indicating decreased activation of osteoblasts, was observed in Dex-PLGA/PBMP treated groups. Collectively, these results demonstrate that PLGA/PBMP microparticle system has great potential for the treatment of CRS-related osteitis by localized corticosteroid delivery on the exposed bones with minimal side effects.

Poster Presentation : **LIFE.P-335**

Life Chemistry

Event Hall FRI 11:00~13:00

Preparation of multimeric rolling circle transcription product with alternating HER1-against RNA aptamer and shRNA and its applications to the specific and efficient delivery into HER1-overexpressing breast cancer cells

Simjeong Koo, Sang Soo Hah[*]

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RNA, one of the major biological molecules, is an attractive material for fabrication of nanostructures in consideration of recent advancements in RNA chemistry, RNA biology and RNA nanotechnology. In addition, rolling circle transcription (RCT), an isothermal enzymatic RNA amplification method, enables self-assembly of multimeric RNA nanostructures from a circular DNA template, which has emerged as one of the fascinating approaches for RNAi-based therapies. In this study, multimeric RCT products containing alternating HER1-against RNA aptamer and HER1-against shRNA units were used as an efficient shRNA delivery method for enhanced gene silencing. The multimeric RCT products allowed for HER1-against RNA aptamer-mediated intracellular delivery specifically into HER1-expressing cancer cells, leading to significant gene silencing results and the following cell death as compared with the monomeric shRNAs and RNA aptamer delivered into the cancer cells by E-fection. Cell viability assays with MDA-MB-231, HeLa, and SK-BR-3 cells, revealed that the higher expression levels of HER1 on the cell surface, the more sensitive to the multimeric RCT products. These results suggest that the introduction of RNA aptamer units as delivery platforms to the multimeric RCT products facilitates highly efficient target-specific binding and the resulting gene silencing of shRNA in target-overexpressing cells.

Poster Presentation : **LIFE.P-336**

Life Chemistry

Event Hall FRI 11:00~13:00

Discovery of a novel small-molecules STING Activator as Cancer Immunotherapeutics.

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The stimulator of interferon genes (STING) is an endoplasmic reticulum transmembrane protein that is a promising target of immunotherapy for cancer. 2’,3’-cGAMP(cyclic GMP-AMP), a natural STING ligand, is endogenously synthesized by cGAS (cyclic GMP-AMP synthase). After 2’,3’-cGAMP binds to STING, conformational changes of STING protein are induced. Then, TBK1-IRF3 downstream signaling pathway is activated, resulting in the production of type I IFNs and pro-inflammatory cytokines. Therefore, the cGAS-STING pathway plays an important role in activation of innate immunity. However, 2’,3’-cGAMP is rapidly cleaved, restricting its use to intratumoral administration. For this reason, it is necessary to find new STING activators. Thus, we discovered novel small-molecules that activate the STING-TBK1-IRF3 signaling pathway.

Poster Presentation : **LIFE.P-337**

Life Chemistry

Event Hall FRI 11:00~13:00

Activity-based Near-Infrared Fluorogenic Probes for Imaging and Separation of O-GlcNAcase

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Glycosidases, also known as glycoside hydrolase, are related to glycan degradation by cleaving glycosidic bonds in glycans and glycoconjugates. As they play key roles in carbohydrate metabolism of living organisms, it is significantly important to understand functions of glycosidases for in-depth studies of carbohydrates.Here, an activity-based near-infrared fluorogenic probe targeting O-GlcNAcase was newly designed and synthesized. The probe consists of (1) a near-infrared (NIR) dye for less background signals and deeper penetration, (2) a fluoromethyl group as a reactive group to capture the target enzyme via a covalent bond, and (3) an alkyne group as a report tag to separate the enzyme-probe complex by affinity chromatography. The intact probes were non-fluorescent. However, as the target glycosidase cleaved the sugar moiety of the probe and fluoride was liberated from the probe, the enzyme was covalently labeled and inhibited by the probe, which was detected using fluorescence microscopy. Details will be described in the presentation.

Poster Presentation : **LIFE.P-338**

Life Chemistry

Event Hall FRI 11:00~13:00

Discovery of chemical compounds that inhibit the nucleic acid unwinding activity of MERS coronavirus helicase

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Middle East Respiratory Syndrome (MERS) coronavirus helicase/NTPase is an essential protein for virus replication and regarded as an attractive target for antiviral therapy. In this study, I report two novel compounds, galangin and amentoflavone, potently inhibit the dsRNA unwinding activity of MERS coronavirus helicase in vitro. However, no ATP hydrolysis activity was observed with two compounds. We measured the % inhibition by increasing the concentration of the compounds, and IC50 values were determined. We also observed that the compounds did not show cytotoxicity up to 80 μM concentration. These results suggest that the compounds might serve as MERS coronavirus inhibitor.

Poster Presentation : **LIFE.P-339**

Life Chemistry

Event Hall FRI 11:00~13:00

Neuroprotective small molecule SB1617 has effects on Tau proteostasis via anti-neuroinflammatory activity in microglia

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Biophysics and chemical biology, Seoul National University, Korea

[1]*Division of Chemistry, Seoul National University, Korea*

The deposition of Tau aggregates in neurons and its propagation to neighboring neurons or microglia are the well-known risk factors for neurodegenerative diseases. Recently, emerging therapeutic strategies targeting neuroinflammatory activity in microglia have shown significant promise in tau pathology. Here, we aimed to explore the microglia-mediated neuroprotective function of SB1617, previously discovered among our in-house library to effectively suppress neuronal tau aggregation. We revealed that SB1617 inactivates pathogenic (M1-like) microglia, leading to the reduction of pro-inflammatory cytokine secretion via translational regulation. In addition, SB1617 contributes to modulate microglial polarization towards M2 phenotype and phagocytic function. Besides, we described that extracellular pathogenic tau can be degraded via autophagy-associated phagocytosis. Lastly, we employed a traumatic brain injury (TBI) mouse model, which pathophysical signaling progression is involved in the neuroinflammatory responses as well as the development of tau pathology. SB1617 shows beneficial effects on tau proteostasis through microglia-mediated neuroinflammatory activity. In conclusion, the tau proteostasis regulation via microglia surveillance function lead to a better understanding of tauopathies and potentially help with the development of new therapeutic approaches.

Poster Presentation : **LIFE.P-340**

Life Chemistry

Event Hall FRI 11:00~13:00

Artificial Cellular Model as a Bioreactor:Highly Efficient and Sustainable Cell-free Protein Synthesis Using Cell Lysate in a Giant Liposome

Sungwoo Lee, Hyun Park, Sungwoo Jeong[1], Kwanwoo Shin*

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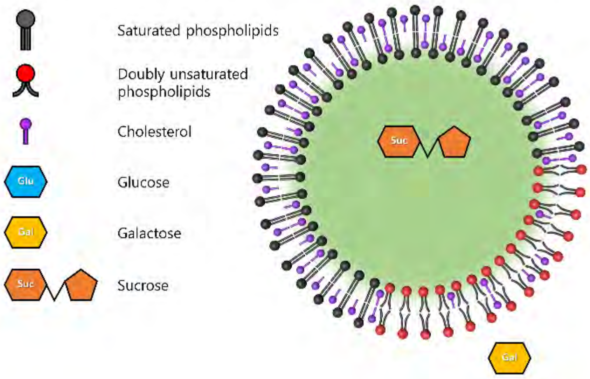
[1]*Research Institute for Basic Science, Sogang University, Korea*

Cell-free protein synthesis (CFPS) based on cell lysate has many advantages over protein synthesis in vivo. In particular, the lack of cell walls allows direct manipulation of biochemical cascades that usually occur in the cytoplasmic space. Meanwhile, we recapitulate that when cell lysate is encapsulated in artificial cell membranes, it could be the ideal cytoplasm for artificial cells capable of protein synthesis and tremendous amounts of biological reactions. It was, however, difficult to implement CFPS reactions using the cell lysates due to the osmotic instability in the confined spaces provided by liposomes and inhomogeneity of the cell lysate. In this research, we developed efficient and sustainable cell lysate-based CFPS system in a giant unilamellar vesicle (GUV). We first selected appropriate sugars for inner and outer buffer to keep the osmotic pressure as low as possible during the whole reaction. For GUV formation, emulsion transfer method was adopted to prepare the cell-lysate encapsulated GUV with high encapsulation efficiency. By applying ultrasound to the vesicles, the homogeneity of the encapsulated cell lysis solution was extremely increased, and as a result, almost all GUVs showed sharp green fluorescence. To keep GUV intact against unpredictable change of osmotic pressure with enhanced stability, saturated lipids and high amounts of cholesterol were added with lipid phase separation. Finally, we successfully fabricated artificial cells as a bioreactor, which are feasible to synthesize various proteins inside using a lysate-based expression system and possible to last for 14 hours at which the reaction in vitro reaches the plateau.


Saturated phospholipids
Doubly unsaturated phospholipids
Cholesterol
Glu
Glucose
Gal
Galactose
Suc
Sucrose
Suc
Gal

Poster Presentation : **LIFE.P-341**
Life Chemistry
Event Hall FRI 11:00~13:00

Design and Synthesis of a Combinatorial Library of DNA-Encoded Bicyclic Peptoids

Kang ju Lee, Min Hyeon Shin, Hyun-Suk Lim*

Department of Chemistry, Pohang University of Science and Technology, Korea

Macrocyclic peptidomimetics have received great interest as a rich source of ligands for target proteins. Among them, owing to their promising properties, bicyclic peptoids are of particular interest. They are anticipated to provide greater structural rigidity and be able to bind far more tightly to targets, even compared to monocyclic peptoids. In addition, given that they possess an unnatural backbone structure (N-substituted glycines), bicyclic peptoids are probable to have improved proteolytic stability and cell permeability compared to native peptides. Despite their high potential as protein capture agents, the construction and screening of combinatorial bicyclic peptoid libraries have been rarely reported.In this presentation, we describe the design and synthesis of a DNA-encoded library of bicyclic peptoids. We demonstrated that our solid-phase approach is robust and DNA-compatible, affording a large combinatorial library of bicyclic peptoids composed of 5 million molecules with various ring sizes and side chains. Affinity-based screening of this library yielded high-affinity ligands for a target protein, demonstrating the capability of the library as an excellent source of protein ligands. We believe that the DNA-encoded library of bicyclic peptoids will serve as versatile tools that enable the discovery of potent ligands against challenging targets, including intracellular protein-protein interactions.

Poster Presentation : **LIFE.P-342**

Life Chemistry

Event Hall FRI 11:00~13:00

Development of a Potent UBR1 Ligand for Targeted Protein Degradation Through the N-Degron Pathway

Hee Myeong Wang, Hyun-Suk Lim*

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Proteolysis-targeting chimeras (PROTACs) are an attractive technology that induces the degradation of a target protein via the ubiquitin–proteasome system (UPS). PROTACs are heterobifunctional molecules that can bind to both the target protein and E3 ligase simultaneously, thereby leading to polyubiquitination and proteasomal degradation of a target. However, despite its great utility as a tool to identify therapeutic candidates, general applications of current PROTACs has been limited. While there are over 600 E3 ligases in the human genome, only a few E3 ligases are targeted by current PROTACs, which are overexpressed in cancer cells (e.g., CRBN and VHL). As a result, most PROTACs have been developed for cancer therapy. To circumvent such restriction, we recently developed a new class of PROTACs based on the N-degron pathway. The N-degron pathway is a proteolytic system that utilizes N-recognins (e.g., UBR1 E3 ligase) to recognize N-terminal residues of proteins (called N-degrons). In contrast to the E3 ligases targeted by current PROTACs, UBR1 is ubiquitously expressed in most cells, and thus PROTACs based on the N-degron pathway could degrade proteins irrespective of cell type. In this study, we developed a potent UBR1 ligand, UL-101, with excellent binding affinity, cell permeability and proteolytic stability. To show that the developed UBR1 ligand can be used for effective degradation of target proteins, we generated a proof-of-concept PROTAC, UL-101-JQ1, by linking the UBR1 ligand to a BRD4 binder, JQ1. Notably, UL-101-JQ1 showed an extensive degradation of BRD4 at nanomolar level, successfully demonstrating that UL-101 can be exploited for developing effective PROTACs. This type of PROTACs could be generally applicable for targeting a wide range of diseases.

Poster Presentation : **LIFE.P-343**
Life Chemistry
Event Hall FRI 11:00~13:00

Fluorescence-Quenching Screen for Discovery of Protein–Protein Interactions Inhibitors

Min hyeon Shin, Hyunsoo Lee[1], Hyun-Suk Lim[*]

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[1]*Department of Chemistry, Sogang University, Korea*

Protein–protein interactions (PPIs) are involved in wide range of biological processes, and aberrant PPIs are implicated in many complex diseases such as cancer and immune-related disease. Hence, there is a significant interest in developing molecules that can modulate disease-related PPIs. However, targeting PPIs is one of the most difficult challenges in drug discovery due to the lack of efficient high throughput screening (HTS) method. The conventional screening methods used for identifying modulators of PPI such as surface plasmon resonance, Förster resonance energy transfer, and enzyme-linked immunosorbent assays are usually based on multi-well plate format. Therefore, they have limitation that the limited number of chemicals could be used in screening. On the other hands, the affinity-based on-bead screen method enables a large number of library molecules (more than millions) to be screened simultaneously. However, on-bead screen methods have inherent false positive problems. The high ligand density on the bead surface enables the target protein to bind with multiple ligands on bead surface (avidity effect), and the hit compounds isolated from screening may not act as inhibitors of PPI, as expected. In this this study, fluorescence-quenching on-bead screen method was firstly developed for discovery of direct inhibitors of target PPI. This system used chromophore labeled target protein and quencher labeled ligand in on-bead screening. By utilizing fluorescence-quenching on-bead screen, we successfully discovered the direct inhibitors of nuclear receptor coactivator 1 and signal transducer and activator of transcription 6 interaction. Taken together, fluorescence-quenching on-bead screen will serve as a novel HTS method for discovering direct inhibitors of PPI excluding false positive issues in typical affinity-based screening.

Poster Presentation : **LIFE.P-344**

Life Chemistry

Event Hall FRI 11:00~13:00

Implementation of Grignard Reaction in DNA-Encoded Library

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Department of Chemistry, Pohang University of Science and Technology, Korea

The DNA-encoded library (DEL) is a set of chemical compounds conjugated with DNA fragments that have synthetic information. It can be used to investigate a much deeper and larger chemical space more cheaply and efficiently than traditional high-throughput-screening, but DNA isn't soluble in organic solvents and can be damaged by several chemicals. This restricts the range of applicable reactions, limiting the chemical space of DEL. Therefore, development of DNA-compatible reactions is essential to make various chemical compounds. In this work implementation of Grignard reaction in solid-phase DEL that cannot be realized in conventional aqueous DEL is described. This study may broaden chemical diversity in DEL, so it may contribute to finding various hit compounds.

Poster Presentation : **LIFE.P-345**
Life Chemistry
Event Hall FRI 11:00~13:00

Development of Novel *In Situ* Click Chemistry Methods for Rapid Discovery of Potent Protein Ligands

Minkyung Kim, Min Hyeon Shin[1], Hyun-Suk Lim[1,*]

Chemistry, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Click chemistry, inducing 1,3-dipolar cycloaddition between alkyne and azide, have attracted much attention in broad research field and also applied in living system, termed as *in situ* click chemistry. Using *in situ* click chemistry, the target protein acts as the biological template and assembles its own ligand by bringing two (or more) moderate affinity of ligands involving clickable sites into close proximity. As a result, the highly potent ligand which is thermodynamically stable and has the most optimized orientation and affinity could be developed. These features allow *in situ* click chemistry to be utilized as the innovative screening method and its efficacy has already been demonstrated by the discovery of various inhibitors.However, in the current screening methods using *in situ* click chemistry, it is technically difficult to cover and prepare the huge diversity of library. This limitation could reduce the chance of discovery of high affinity ligand. To overcome this problem, we choose to construct the chemical library on nanoparticle with huge diversity and DNA tags are used as the encoding material in the screening process. In previous study, we developed the strategy of DNA-encoded one-bead one-compound library and demonstrated its practicability through the affinity-based screening. The synergetic effect between huge diversity of nanoparticle library and screening based on *in situ* click chemistry could provide great improvements in developing the novel and rapid screening method for discoverying of potent protein ligands.Herein, for the first time, we have demonstrated the screening system based on *in situ* click chemistry using nanoparticle library. As the proof of concept study, the anchor ligand, which has low activity against target protein PTP1B, including alkyne moiety was prepared and linear peptoid DNA-encoded library involving azide moiety was constructed on nanoparticle with more than 20 million diversity. Screening based on *in situ* click chemistry was performed by incubating anchor ligand and nanoparticle library with target protein as the catalytic scaffold. From the result of screening, hit compounds showed much more improved inhibition activity and selectivity against to the target protein, compared to the anchor ligand.

Poster Presentation : **LIFE.P-346**

Life Chemistry

Event Hall FRI 11:00~13:00

Evaluation of the Cell Permeability of Bicyclic Peptoids/Peptide-Peptoid Hybrids

Chang Deok Seo, Hee Myeong Wang[1], Hyun-Suk Lim[*]

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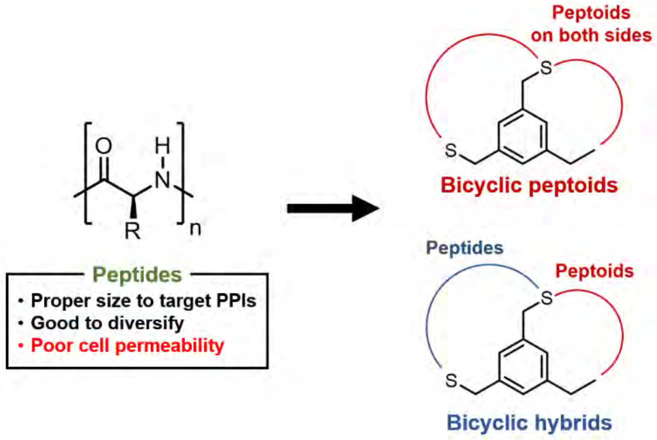
[1]*Pohang University of Science and Technology, Korea*

Peptides have been playing important roles in the field of chemical biology as drugs, probes, and so on. However, natural peptides are easily degraded by proteases and have low cell permeability, so targeting intracellular targets is quite challenging. Recently in our lab, we have systematically investigated that monocyclic peptoids, the N-substituted glycine oligomers, have significantly improved cell permeability compared to linear counterparts. As the improved version, bicyclic peptoids are a promising class of peptidomimetics that are expected to have significantly improved structural rigidity and preorganized structure compared to linear peptides and peptoids. Moreover, bicyclic peptide/peptoid hybrids are promising peptidomimetics that are thought to have the overall advantages of the bicyclic scaffolds, peptides, and peptoids. However, systematic investigation on the cell permeability of these bicyclic peptoids and hybrid structures has not been reported so far. Here, we firstly verified that the cell permeability of bicyclic peptoids is significantly increased compared to their linear counterparts in various ring sizes and side chains. In addition, the cell permeability of the bicyclic hybrids was also demonstrated to be superior to that of the linear peptides. This improvement of cellular uptake efficiency was confirmed to be a synergetic outcome of the bicyclic structure and the peptoid characters. Through this study, we showed that cell-permeable bicyclic peptoids and bicyclic hybrids could be developed as prominent molecules targeting intracellular proteins.


Peptides
• Proper size to target PPIs
• Good to diversify
• Poor cell permeability
O
H
N
R
n
Peptoids
on both sides
S
S
Bicyclic peptoids
Peptides
Peptoids
S
S
Bicyclic hybrids

Poster Presentation : **LIFE.P-347**

Life Chemistry

Event Hall FRI 11:00~13:00

Discovery of Small Molecule Ligands of GID4 for the N-Degron mediated PROTACs

Jae Sub Kim, Min Hyeon Shin, Hyun-Suk Lim[*]

Department of Chemistry, Pohang University of Science and Technology, Korea

PROTAC(proteolysis-targeting chimera) is an emerging therapeutic strategy with the potential to tackle disease-causing proteins that have historically been highly challenging to target with conventional small molecules. The PROTACs are perceived as promising therapeutic strategy because of the potential to overcome the limitation of conventional therapeutics, and many research groups and global pharmaceutic companies are intrigued to this technology. However the PROTACs have some limitations that only a handful of E3 ligases(cereblon, VHL, etc.) of over 600 E3 ligases in human body are used in current PROTAC design and they are overexpressed only in cancer cells. So the current PROTACs cannot be used in cells or tissues that not express those of E3 ligases, and it is difficult to target diverse intractable disease except for cancers. So, the urgent unmet need in PROTAC technology is development of generally applicable PROTAC system. For this, PROTACs that exploit N-degron pathway(N-Degron pathway targeting chimeras, NDTACs) were devised. The N-degron pathway is a proteolytic system in which the N-terminal amino acids of short-lived proteins are recognized by the certain E3 ligases like GID4. Given that the N-degron pathway is ubiquitously expressed in most cells, PROTAC using the GID4 as E3 ligase could degrade a protein of interest regardless of cell and tissue types.Inhere, I discovered novel small molecule GID4 ligands by mimicking the structure of tetrapeptide ligand of GID4. They showed enhanced binding affinity and cell permeability than the initial peptidic ligand. So, it is expected to be used in novel NDTACs which have good cellular activity and general applicability in many intractable diseases like obesity, diabetes, neurodegenerative diseases.

Poster Presentation : **LIFE.P-348**

Life Chemistry

Event Hall FRI 11:00~13:00

Structure-activity relationship of activity-based probes targeting the high-temperature requirement A (HTRA) serine proteases

Jiyu Lee, Jiyoun Lee[1,*], Eunchae Park[2]

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The high temperature requirement A (HTRA) family of serine proteases mediates protein quality control. These proteins process misfolded proteins in several diseases including Alzheimer’s disease (AD) and Parkinson’s disease (PD). While their structures and activation mechanisms have been studied, the precise details of the regulation of their activity in physiological conditions have not been completely elucidated, partly due to the lack of suitable chemical probes. We have previously developed a series of activity-based probes selectively targeting the HTRA family of proteases including HTRA1, HTRA2 and DegP. In this work, we optimized the previously developed tetrapeptide probes by incorporating non-natural amino acid residues to improve selectivity and specificity. We evaluated selectivity of our novel series of probes by using various recombinant serine proteases and established structure-activity relationship.

Poster Presentation : **LIFE.P-349**
Life Chemistry
Event Hall FRI 11:00~13:00

Spatiotemporal protein crosslinking by light activation (Spotlight) for in-vivo interactome mapping.

Pratyush Mishra*, Hyun-Woo Rhee[1,*]

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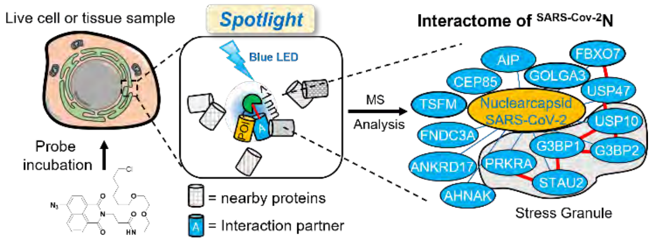
To identify the interactome of POI in live cells, Among the various chemical labeling and chemical crosslinking methods which have been combined with mass spectroscopy, photo-crosslinking method have provided in vivo protein-protein interaction partner in live cells with less perturbation to the cellular physiology. However it is still very hard to genetically introduce photo-reactive groups to the POI. Furthermore, many photo-crosslinkers are designed to be activated by ultraviolet (UV) light which causes photo-toxicity and suffers from low tissue penetration. Herein, we developed a visible light activable fluorescent photo-crosslinking ligand which can be genetically introduced to the POI-conjugated HaloTag. Its ability to crosslink physically interacting proteins was confirmed by covalently capturing a rapamycin-induced protein interaction between FK506 binding protein (FKBP) and the FK506-rapamycin binding (FRB) domain in living cells under the presence of rapamycin , probe and visible light activation. Our method successfully captures stress induced proteome change as well as enables photocrosslinking in tissue samples. Since our method is orthogonal to current proximity labeling methods, we also confirmed that our method can be compatibly utilized with TurboID (Spotlight-Turbo). Using Spotlight, we attempt to identify the host interactome of Nucleocapsid (N) protein of SARS-CoV-2, which is essential for viral genome assembly process. From the mass analysis of the VL1-crosslinked product of N-HaloTag in HEK293T cells, RNA binding proteins in stress granule and P-body proteins were enriched in the crosslinked samples. From follow-up study, we confirmed that our method can reveal the specific interactome of N protein within a few angstrom distance in live cells


Live cell or tissue sample
Spotlight
Blue LED
POI
A
Probe incubation
N_3
O
N
O
HN
O
O
= nearby proteins
A = Interaction partner
MS Analysis
Interactome of SARS-Cov-2N
AIP
FBXO7
CEP85
GOLGA3
USP47
TSFM
Nuclearcapsid SARS-CoV-2
USP10
FNDC3A
G3BP1
G3BP2
ANKRD17
PRKRA
STAU2
AHNAK
Stress Granule

Poster Presentation : **LIFE.P-350**

Life Chemistry

Event Hall FRI 11:00~13:00

Activated furans as colorimetric and ratiometric amine sensors

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Amines are an important class of functional groups in the biological system as well as in the synthetic world because of their extra pair of electrons. The unique chemical reactivity of amines is widely recognized in industry, and organic amines are one of the most utilized chemicals in pharmaceutical manufacturing and materials processing. Methods to detect and quantify the biogenic amines are useful in many aspects from disease diagnostics to food quality control. Among the currently available detection platforms for biogenic amines, colorimetric chemosensors enabling naked-eye detection would provide a fast and easily accessible detection method. MAF has been mostly used as a precursor to make molecular photoswitches, because it can be readily incorporated into a chromophore to exert donor-acceptor photoswitching. MAF-based amine sensors undergo characteristic color changes upon reacting with amines. Inspired by these approaches, we developed a series of MAF-based chromogenic sensors to detect organic amines. In this work, we examined sensitivity and selectivity of these MAF-based probes and also tested their potential applications as a readily available paper-based sensing system.

Poster Presentation : **LIFE.P-351**

Life Chemistry

Event Hall FRI 11:00~13:00

A chemoenzymatic system for fluorescent signal amplification using genetically encoded peroxidase (FLEX) in live cells

Nirmali Sharma, Hyun-Woo Rhee[1,*]

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Recently, peroxidase-based reactions are being more popular in the cellular biology. In these method, genetically encoded peroxidases (APEX or HRP) generate short-lived radicals and they can be used for extraction of local proteome in-formations or image the specific protein in higher resolution using electron microscope (EM). We developed a modular strategy using a phenolic probe which generates fluorescence after peroxidase reaction and can be subsequently imaged in nanoscale resolution using electron microscope. Since APEX has already well-developed libraries for APEX2-POI (protein of interest) across the globe, using this fluorescent phenolic probe can be of immense help for deciphering the ultrastructure as well as fluorescence localization of protein of interest using CLEM.

Poster Presentation : **LIFE.P-352**
Life Chemistry
Event Hall FRI 11:00~13:00

Targeted Degradation of Transcription Coactivator SRC-1 through CRBN-based PROTAC

So Ra Choi, Min Hyeon Shin, Hyun-Suk Lim*

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Abnormally activated steroid receptor coactivator-1 (SRC-1) expression and activity are strongly correlated with cancer progression and metastasis. Here we report the development of a proteolysis targeting chimera (PROTAC) that is composed of a selective SRC-1 binder linked to a specific ligand for cereblon (CRBN). We showed that the bifunctional molecule efficiently and selectively induced the degradation of SRC-1 in cells through CRBN-based PROTAC. Targeted protein degradation mediated by PROTACs represents a novel therapeutic opportunity for potential therapy that selectively targets proteins for removal from cells by the ubiquitin–proteasome system (UPS). PROTACs act in a catalytic manner, and this strategy has great potential to target many challenging proteins. In our previous work, we successfully utilized the N-degron pathway-based PROTAC technology for selective degradation of SRC-1. However, PROTACs based on the N-degron pathway have a few additional hurdles to overcome as many peptide-derived drugs do such as in vivo instability and membrane impermeability. Thus, as an alternative strategy to overcome intrinsic disadvantages of peptide PROTACs, herein we propose the CRBN-mediated degradation of SRC-1. CRBN ligand offers several important advantages in respect to cellular uptake efficiency and proteolytic stability, leading to rapid target degradation. Importantly, we designed and synthesized bifunctional molecules consist of a selective SRC-1 ligand and CRBN ligand moiety, thereby able to recruit the E3 ligase to induce protein degradation. As expected, PROTACs targeting the CRBN exhibited the most potent activity in reducing cellular SRC-1 levels in a dose-dependent fashion. Together, these results demonstrate that the SRC-1 degrader can be an invaluable chemical tool in the studies of SRC-1 functions.

Poster Presentation : **LIFE.P-353**

Life Chemistry

Event Hall FRI 11:00~13:00

Constructing the artificial photosynthetic organelle using microbial rhodopsin

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[1]*Chemistry, Sogang University, Korea*
[2]*Research Institute for Basic Science, Sogang University, Korea*

Photosynthesis is the most important process for the survival of living organisms and is a system used by plants or other organisms to convert light energy into chemical energy. In photosynthetic bacteria, the proteins that gather light for photosynthesis are embedded in the cell membrane. Such proteins are transmembrane proteins that extend through a bilayer of lipid within the cell and acts primarily as a conduit for chemical material transport. Until now, several protein reconstitution protocols were developed and suggested to reconstitute transmembrane proteins into the artificial cell, but the efficiency and stability of the membrane proteins in artificial cellular membranes still need to be further improved. In this study, we developed an artificial photosynthetic cellular model with microbial rhodopsin to find a way to improve reconstitution efficiency. The efficiency of transmembrane protein insertion was measured under a wide variety of conditions such as lipid compositions, pH, temperature, cholesterol ratios, and buffer conditions. To confirm the functional activity of microbial rhodopsin in artificial cells, the expression of microbial rhodopsin was measured by a pH indicator, carboxyl SNARF-1, in the rhodopsin reconstituted liposome. This model may provide an optimal way for constructing various functions of transmembrane in artificial cell models. Also, understanding photosynthesis using this artificial cell can be point the way to improve various understanding the origin of life and energy applications.Keywords: artificial cell, protein reconstitution, transmembrane protein, microbial rhodopsin

Poster Presentation : **LIFE.P-354**

Life Chemistry

Event Hall FRI 11:00~13:00

Finding Threshold of Cytoplasmic Protein Structures in Mammalian Cells Using Super-resolution Microscopy

Sang Ho Lee, Albertus Ivan Brilian[1], Chang Ho Kim[2], Kwanwoo Shin[*]

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[1]*Chemistry, Sogang University, Korea*
[2]*Institute of Biological Interfaces, Sogang University, Korea*

Cytoskeletal proteins provide mechanical tensions within cells that regulate critical cellular functions. While many techniques explored protein deformations on a macroscale, only few focused on the mechanosensing on a nanoscale. Furthermore, the threshold limit of cytoskeletal proteins still remains unclear. Using super-resolution microscopy and a manual cell stretching device, actin fibers of a human dermal fibroblast were unidirectionally pulled until nanoscale deformations were observed. Microcontact printing and patterning techniques were also implemented to ensure consistent control of cytoskeletal widths of the fibroblasts. Stimulated emission depletion microscopy (STED) allowed observing subdiffractional tears that were once immeasurable using conventional confocal microscopy, and the elastic deformation of the substrate enabled finding the minimum threshold mechanical force needed to make nanoscale deformations in the adherent cell. Measurement of mechanical limitation of cytoskeletal proteins in nanoscale also aids in predicting their mechanoresponsive behaviors on a macroscopic level.

Poster Presentation : **LIFE.P-355**

Life Chemistry

Event Hall FRI 11:00~13:00

A study on antimicrobial peptoids including metal-chelating moiety that generates reactive oxygen species.

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Antimicrobial peptides (AMPs) derived from nature show broad-spectrum antimicrobial activity, drawing attention as a candidate to replace traditional antibiotics. Most AMPs directly target and disrupt bacterial cell membranes, potentially avoiding the resistance mechanisms of the antibiotics—however, the susceptibility to proteolytic degradation limits AMPs with their local administration route. Peptoids are peptidomimetics that potentially overcome peptides' stability issues, but they also have room to improve efficacy and selectivity for clinical use. In this study, we introduced metal chelating moieties known to generate reactive oxygen species to enhance the potency of antimicrobial peptoids. We prepared a library of peptoids with metal chelating moieties and evaluated antimicrobial activity and cytotoxicity compared to the parent peptoid. In addition, the antimicrobial mechanism of the peptoids was investigated.

Poster Presentation : **LIFE.P-356**

Life Chemistry

Event Hall FRI 11:00~13:00

Circularly polarized luminescence active pyrene-containing peptoids

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Circularly polarized light shows promise in future displays and photonic technologies. Circularly polarized luminescence (CPL) from chiral luminophores is an effective method for producing circularly polarized light. CPL active peptoids were synthesized. Chiral pyrene-based peptoid submonomer was synthesized with Ellman’s auxiliary. Pyrene-containing peptoids were synthesized in solution using a submonomer synthesis technique. Pyrene-containing peptoids were (+)CPL active in the early stages of elongation; however, as the peptoid acquired secondary structure as a polyproline type-I (PPI) like helix, chiroptical properties were inverted. The photophysical properties of pyrene-containing peptoid were determined with UV-vis, fluorescence spectroscopies, and lifetime measurement. Circularly polarized luminescence efficiency (g_{lum}) was comparable to that of chiral organic dye (~10^{-3}) with low concentration (10 μM).

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **LIFE.P-357**
Life Chemistry
Event Hall FRI 11:00~13:00

Development of a fluorescent nanosensor for monitoring mRNA expression and its application

Yeajee Yim, Dal-Hee Min*

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Due to the coexistence of graphene-like hydrophobic domain and various oxygen-containing groups, graphene oxide (GO) shows a strong affinity towards single-stranded nucleic acid and fluorescence quenching capability induced by fluorescence resonance energy transfer. The preferential binding of GO to single-stranded nucleic acid over double-stranded nucleic acid provides a basic principle of various GO-based biomolecule detection platforms, resulting in the change of fluorescence signal. However, despite the presence of improved platforms, mRNA detection is still challenging because of the long length and secondary structure of mRNA. Here, we present a fluorescent nanosensor system for monitoring mRNA expression. GO-based fluorescence sensing successfully shows a sequence-specific signal in living cells that produce target mRNA. With the operational simplicity and sensitive detection performance, our system exhibits great potential to be applied in live-cell screening for the primary selection of genetically modified cells.

Poster Presentation : **LIFE.P-358**

Life Chemistry

Event Hall FRI 11:00~13:00

FRET-based amino acids sensors using a fluorescent amino acid as a FRET donor

Sang Won Lee, Hyunsoo Lee*

Department of Chemistry, Sogang University, Korea

FRET sensors based on fluorescent proteins have been powerful tools for probing protein–protein interactions and structural changes within proteins. However, they are intrinsically limited by their large size and the requirement for N- or C-terminal fusions. In this report, a FRET-based sensor was developed by incorporating a fluorescent unnatural amino acid into periplasmic binding proteins (PBPs), which formed a FRET pair with fluorescent proteins (FPs). GFP or YFP was fused to the N-terminus of PBPs, and the fluorescent unnatural amino acid was incorporated into a specific site in PBPs. Sensor proteins were designed for Gln, Leu, and Met, and they produced a 2 to 3-fold increase in the FRET ratio upon target amino acid binding, whereas either no change or minimal change was seen using other amino acids, including the other 19 natural amino acids. This novel design strategy for FRET sensors overcomes the limitations of current FRET sensors, which require the use of two fluorescent proteins. Consequently, our strategy may prove useful for investigating protein–protein interactions and for probing changes in protein conformation.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **LIFE.P-359**

Life Chemistry

Event Hall FRI 11:00~13:00

Protein Dimerization Using a Genetically Encoded Metal-Chelating Amino Acid

Sooin Kim, Hyunsoo Lee[1,*]

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[1]*Department of Chemistry, Sogang University, Korea*

Many natural proteins function in oligomeric forms, which are critical for their sophisticated functions. The construction of protein assemblies has great potential for biosensors, enzyme catalysis, and biomedical applications. In designing protein assemblies, a critical process is to create protein–protein interaction (PPI) networks at defined sites of a target protein. Although a few methods are available for this purpose, most of them are dependent on existing PPIs of natural proteins to some extent. In this report, a metal-chelating amino acid, 2,2′-bipyridylalanine (BPA), was genetically introduced into defined sites of a monomeric protein and used to form protein dimers. To develop a general strategy for protein dimerization, BPA was introduced into multiple sites of a model protein, maltose binding protein (MBP), and each mutant MBP was analyzed to test if they dimerize in the presence of a metal ion. Two different species of metal ions (Ni^{2+} and Cu^{2+}), were found to have the ability to make a protein dimer. Moreover, the important factor for the protein dimerization was the location of the site where BPA is incorporated. In addition to making a homodimer protein complex, engineering the sites for BPA incorporation makes it possible to construct a heterodimer protein complex. The method proposed in this report is technically simple and generally applicable to various proteins with interesting functions. Furthermore, a heterodimer complex could be used for two different enzymes which also leads to the substrate channeling technique. Therefore, this method would be useful for the design and construction of functional protein assemblies.

Poster Presentation : **LIFE.P-360**

Life Chemistry

Event Hall FRI 11:00~13:00

Ultrashort antimicrobial peptoids with *C*-terminal modifications

Heewoong Yoon, **Jiwon Seo***

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Natural lipopeptides are produced nonribosomally by bacteria and fungi during the growth on various carbon sources. Some of them have potent antimicrobial activity; polymyxin B and daptomycin have been used to treat infectious diseases caused by gram-negative and gram-positive bacteria, respectively. Despite the potent activity against pathogenic bacteria, many natural lipopeptides are cytotoxic to mammalian cells. Ultrashort peptides have attracted considerable interest as an alternative to natural peptides due to their low cytotoxic activity, high efficiency, and lower cost of manufacture. In this study, we designed and synthesized *C*-terminal modified ultrashort peptoids, and carried out a structure-activity relationship (SAR) study. The peptoids possess excellent antimicrobial activity and enhanced cell selectivity, and there were differences in biological activity based on the peptoid sequence and *C*-terminus motif. These results suggest that ultrashort peptoids have strong potential as a new class of novel antibiotic therapeutics.

Poster Presentation : **LIFE.P-361**

Life Chemistry

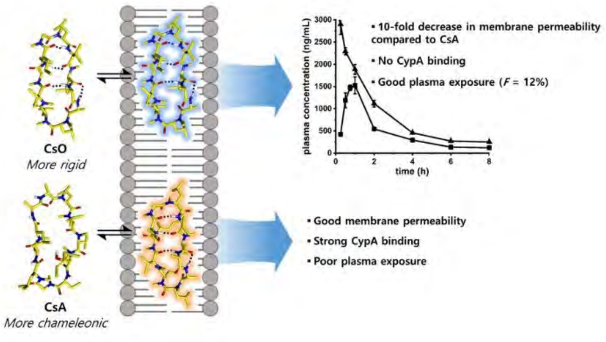
Event Hall FRI 11:00~13:00

Evaluation of chameleonic behavior of macrocyclic peptide cyclosporin O scaffold and its effect on membrane permeability, cyclophilin A binding, and pharmacokinetic profile

Dongjae Lee, Jiwon Seo*

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

The chameleonic behavior has been emerged as a key conformational property to achieve high membrane permeability and oral bioavailability for macrocyclic peptides in the beyond rule of five (bRo5) chemical space. Some natural or synthetic products (e.g., cyclosporin A (CsA)) were investigated to understand the chameleonic behavior and identify the structural features, but general guidelines to design chameleonic molecules are still unknown. In this study, the chameleonic behavior of cyclosporin O (CsO) and its derivatives modifying the side chains was evaluated by NMR spectroscopy, and its effect on membrane permeability, cyclophilin A (CypA) binding, and the pharmacokinetic profile was described. CsO showed weaker chameleonic behavior than CsA even though a similar closed conformation was observed for CsA and CsO. The weaker chameleonic behavior of CsO explained the decrease in membrane permeability and CypA binding. It led to a higher plasma concentration and moderate oral bioavailability (*F* = 12%). We believe that CsO scaffold can afford insight into understanding the chameleonic behavior and designing membrane permeable and orally bioavailable drugs in the bRo5 chemical space.



- 10-fold decrease in membrane permeability compared to CsA
- No CypA binding
- Good plasma exposure (*F* = 12%)

- Good membrane permeability
- Strong CypA binding
- Poor plasma exposure

Poster Presentation : **LIFE.P-362**

Life Chemistry

Event Hall FRI 11:00~13:00

Post-synthetic method for introducing multiple azole moieties on side chains of peptoids

Jiwon Seo*, Yen Jea Lee

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Natural metalloenzymes utilize multiple imidazole moieties to stabilize metal centers. Incorporating multiple azole moieties into ligands, inspired by nature's design principle, has been regarded as an effective way to construct transition metal complexes. Herein, we demonstrate how to insert multiple azoles on the side chains of peptoids via a simple substitution reaction involving azoles (imidazole, pyrazole, 1,2,3-triazole, and tetrazole) and a chloroalkyl-containing peptoid. As a result, ten azole-containing peptoids were synthesized from a single chloroalkyl-containing peptoid, and the efficiency of each azole in the substitution reaction was examined. We have found that several azole-containing peptoids are capable of binding with Cu(II) and Fe (III). Our synthetic method can contribute to the chemical diversity of peptoids and the development of novel peptoids for metal recognition and catalysis.

Poster Presentation : **LIFE.P-363**

Life Chemistry

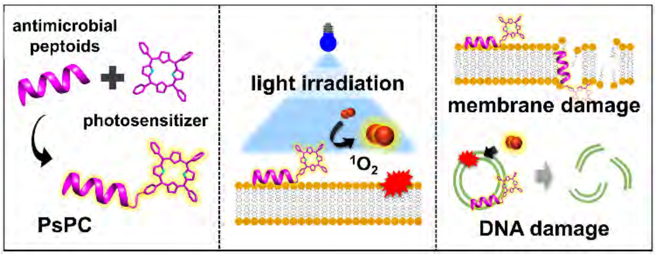
Event Hall FRI 11:00~13:00

Photosensitizer-peptoid conjugates: multitargeting antimicrobial photodynamic therapy agent

Jiwon Seo*, Woojin Yang

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

Multitarget antimicrobials have shown promising activity because they minimize the resistant development of bacteria, and are thus considered in the clinic. Here, we prepared the conjugates of antimicrobial peptoids and photosensitizers that show multitargeting antimicrobial activity. A library of photosensitizer-peptoid conjugates (PsPCs) was synthesized using solid-phase methods, and the structure-activity relationship was studied by employing different peptoid structures, linkers, and photosensitizers. PsPC 9 exhibited the most promising photoresponsive activity among the synthesized PsPCs, which consists of weakly helical peptoids, glycine linkers, and positively charged porphyrins. It was confirmed by spectroscopic analyses that the singlet oxygen was generated upon the excitation of PsPC 9 with blue light. Further studies with flow cytometry and DNA gel electrophoresis demonstrated that PsPC 9 could damage the bacterial membrane and plasmid DNA of gram-negative bacteria. The promising photoresponsive activity of PsPC 9 suggests that an optimal combination of peptoids and photosensitizers provides an efficient antimicrobial photodynamic therapy agent with a multitargeting strategy.



Poster Presentation : **LIFE.P-364**
Life Chemistry
Event Hall FRI 11:00~13:00

Noninvasive characterization of protein-protein interactions by FRET imaging in living cells

Soojung Yi, Nam Ki Lee[1,*]

Department of Chemistry, Seoul National University, Korea
[1]*Division of Chemistry, Seoul National University, Korea*

Protein-protein interactions (PPIs) play crucial roles in most biological processes including gene expression, DNA replication and repair, signal transduction, and cellular metabolism. One of the most important parameters to characterize PPIs is the dissociation constant (K_D), which reflects the strength of PPIs. Measurement of K_D *in vitro* is relatively feasible since the concentration of proteins and their environment can be easily controlled. In contrast, it is challenging to characterize PPIs within intact cells due to the cellular complexity and the absence of a noninvasive method of quantifying intracellular proteins. Despite the difficulties, the importance of investigating PPIs *in vivo* has been increasing because the two environments differ greatly. Here, we established three-channel fluorescence resonance energy transfer (FRET) imaging system and directly obtained K_D of PPIs in single living cells, which has been considered a challenging task. The identification of the PPIs in living cells can provide us with a better understanding of the intracellular environment.

Poster Presentation : **LIFE.P-365**

Life Chemistry

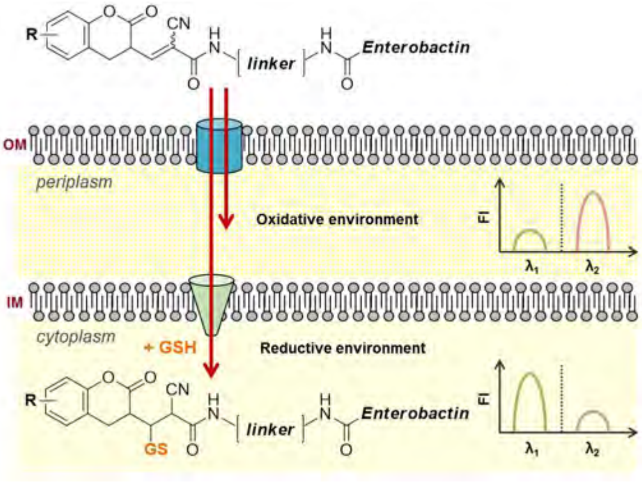
Event Hall FRI 11:00~13:00

Study on a systematic method for cytoplasmic delivery of siderophore conjugates with fluorescent probe

Heeyeong Lee, Hak Joong Kim[1,*]

Chemistry, Korea University, Korea
[1]*Department of Chemistry, Korea University, Korea*

Siderophore-antibiotic conjugate, "SAC", is one of a method to break through antibiotic resistance in Gram-negative bacteria. Pharmaceutical companies have used a simple bidentate chelator, catechol or ortho-pyridone, as drug carriers, as in the example of cefideracol. In this case, antibiotics available are limited because they cannot pass through the endometrium when administered to gram-negative bacteria, allowing drug delivery only to periplasm. On the other hand, it has been reported that drugs can be delivered to cytoplasm in natural SAC, as in examples of albomycin. However, there are still a few examples of success, and the pattern varies depending on the type of siderophores. Accordingly, it is necessary to develop a systematic method for delivering drugs to cytoplasm using natural siderophores.In this poster, fluorescent probes were proposed to systematically test the possibility of transmission in the Gram-negative bacterial cytoplasm of a specific composite design. The drug delivery destination is determined by siderophores, junction sites, and linkers. Based on the difference in the cellular environment in which the cytoplasm is a reducing environment rich in glutathione (GSH), whereas the periplasm is oxidative environment, the probe library was designed as a structure capable of changing optical characteristics. Enterobactin, a kind of siderophore used by Gram-negative pathogens was connected to fluorescent probe through various linkers. After the synthesized probe was treated on cells, a structure capable of cytoplasmic delivery was derived through fluorescence microscopy and flow cytometry analysis. Based on this study, it is hoped that it can be helpful in discovering SAC effective substances that actually target cytoplasm.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periplasm
Oxidative environment
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λ_1
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+ GSH
Reductive environment
R
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GS
linker
Enterobactin
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λ_2

Poster Presentation : **LIFE.P-366**

Life Chemistry

Event Hall FRI 11:00~13:00

Covalent Writing of Single DNA Molecules using AFM

Eung-Sam Kim

Department of Biological Sciences, Research Center of Ecomimetics and Center for Next Generation Sensor Research and Development, Chonnam National University, Korea

In contrast to the conventional top-down microfabrication, bottom-up micropatterning or nanopatterning can be viewed as the localization of target molecules to the desired position of a two-dimensional surface. These processes rely on the physical adsorption of ink-like molecules to the paper-like surface, resulting in unstable immobilization of the target molecules through their noncovalent linkage to the surface. Herein, successive single DNA nick-sealing on a dendron-coated silicon surface allowed us to covalently immobilize individual DNA molecules at defined positions via atomic force microscopy. The covalently-patterned ssDNA that was biotinylated at its terminal was visualized by streptavidin-coated gold nanoparticles. The successive covalent positioning of the target DNA under ambient conditions may facilitate the bottom-up construction of DNA-based nanostructures, nanorobots, or data storage.

Poster Presentation : **LIFE.P-367**

Life Chemistry

Event Hall FRI 11:00~13:00

New building block for effective synthesizing of cysteine contained signature peptide

Suyeon Yeom, Hak Joong Kim[1,*]

Chemistry, Korea University, Korea

[1]*Department of Chemistry, Korea University, Korea*

The selection and synthesis of signature peptides of candidate proteins is very important in multiple reaction monitoring (MRM) technique1), which enables sensitive and accurate quantitative analysis of peptides and proteins. When select the signature peptides, labile or reactive amino acid residues should be avoided. Among them, cysteine is one of the unstable amino acid because sulfhydryl group is easily oxidized. 2) So, cysteine containing peptides that there was a limitation as a signature peptide. As a method to eliminate intra- or inter-disulfide bond formation of peptides, it is common practice to reduce with DTT treatment and then alkylate with iodoacetamide or iodoacetic acid.3) But during alkylation, side reactions, like overalkylation at others undesired functional group, frequently happen.4) In this presentation, we introduce a new building block, alkylated cysteine, that can overcome the reported problems and stably synthesize a signature peptide containing cysteine.1)Teresa A. Brentnall et al. J.Proteome Res. 2009, 8, 2, 787-7972) Lisa J. Zimmerman et al. Biochemistry 2013 , 52 , 22 , 3797–38063) Wenying Jian et al. Rev Anal Chem 2014, 33,1, 31-47 4) Rong hu et al. Mol. Biosyst., 2017, 13, 2574-2582

Poster Presentation : **LIFE.P-368**

Life Chemistry

Event Hall FRI 11:00~13:00

The role of transcription-translation coupling in *E. coli*

Soojin Park, Nam Ki Lee[1,*]

Department of Chemistry, Seoul National University, Korea

[1]*Division of Chemistry, Seoul National University, Korea*

In prokaryotes, the nascent mRNA emerging from the transcribing RNA polymerase is simultaneously translated by ribosomes, which leads to the functional coupling of transcription and translation processes. Transcription-translation coupling (TTC) is an important phenomenon that maintains both efficiency and robustness of gene expression in bacterial cells. However, how TTC affects the transcription stages other than elongation is poorly understood. Here, we quantified mRNAs in *E. coli* cells using single-molecule FISH and observed the significant decrease of transcription efficiency without translation, which cannot be fully explained by the previously reported TTC effects. Based on the further studies using translation-regulated mutants and investigation using chip-exo, we suggest a new role of TTC in gene regulation.

Poster Presentation : **LIFE.P-369**

Life Chemistry

Event Hall FRI 11:00~13:00

Site-specific protein labeling using genetic code expansion technology

Hanbin Yi

Sogang University, Korea

Recently various methods have been developed for protein conjugation. In this study, site-specific protein labeling strategies using cycloaddition reactions based on genetic code expansion technology will be discussed. It is technically simple and allows site-specific conjugation. Various reactive functional groups of the unnatural amino acids considered for a site-specific protein conjugation include ketones, azides, alkynes, cyclooctynes, tetrazines, α,β-unsaturated amides, norbonenes, transcyclooctenes, and bicycle[6.1.0]-nonynes. Among conjugation reactions using these functionalities, azide-alkyne cycloaddition and strain-promoted oxidation-controlled cyclooctyne-1,2-quinone cycloaddition are most popular owing to their high efficiency and bioorthogonality. Protein-containing unnatural amino acid with reactive functional groups can be site-specifically labeled with a fluorophore. It also can be useful for constructing protein-protein conjugates by two mutant proteins containing unnatural amino acid.

Poster Presentation : **LIFE.P-370**

Life Chemistry

Event Hall FRI 11:00~13:00

Anlysis of reactive chemical species and its metabolite in animal modell by immuno assay and electrochemiluminescence.

Ji hwan Park, Yecheol Park[1], Sehoon Kim[1,*]

Medical Convergence Engineering, KU-KIST Graduate School of Converging Science and Technology, Korea

[1]*Korea Institute of Science and Technology, Korea*

Recently, numerous studies revealed the correlation between reactive chemical species (RCS), its metabolites, and diverse diseases such as diabetes, Alzheimer's, or atherosclerosis. It indicates that RCS and its metabolites play a role as important candidates for biomarkers that can be used for the pre-diagnosis of fatal diseases. However, short lifetime, small size, and various interactions with protein interfere with RCS and the detection of its metabolites in the blood. To verify the level of RCS and its metabolite in blood, we constructed a coronary artery disease, hyperlipidemia, diabetes mellitus model and conducted an enzyme-linked immunosorbent assay (ELISA). Finally, we successfully selected the most disease-relevant essential analyte, and develop the immuno-electrochemiluminescence(immuno-ECL) system for sensitive detection of the analyte in blood

Poster Presentation : **LIFE.P-371**

Life Chemistry

Event Hall FRI 11:00~13:00

The effect of improving anti-obesity and liver function of *colocasia esculenta* extract containing polysaccharide

Dong-woo Kang, In-Ah Lee[1,*]

Chemistry, Kunsan National University, Korea

[1]*Department of Chemistry, Kunsan National University, Korea*

Colocasia esculenta is known by many researchers to have excellent efficacy in anticancer. this study attempts to prove the usability of improving obesity using *Colocasia esculenta* (CE), and the CE water extract(CEW), and the CE polysaccharide(CEP). Obesity is accompanied by disproportionate parts of the body and inflammation. In recent studies, the anti-obesity effects of CEW and CEP on 8 weeks of a high-fat diet were investigated. CE, which is effective in anticancer, showed efficacy in inflammation. In particular, as a result of confirming the effectiveness of improving obesity through animal experiments using polysaccharides, it was confirmed that the indicators of obesity were suppressed.In addition, the components of polysaccharides in CE were confirmed using an amino acid analyzer, and additional parts were confirmed through device analysis. the weight of liver, fat, and colon tissues after obesity induction was measured, and the weight of tissues was decreased in the CE group compared to the control group. In addition, the plasma of experimental animals showed 39.32% lower triglycerides in the CE group than the control group, but 28.43% increase in HDL cholesterol. As a result of checking various inflammation levels using PCR and ELISA, the high-fat diet in CPT-1 showed 43.48% difference in the control group and CEW and 24.78% difference in CEP, and 32.36% and 13.34% lower in SREBP, respectively, and the effect of lowering factors related to obesity and inflammation such as HSL, iNOS, FAS, ACC-1, UCP-1, PPARγ, CEBPα, FABP4, and LXR was confirmed. The biochemical analyzers such as ALT, AST, LDL, and BUN will be used to confirm the activity, kidney function activity, protein degradation of liver enzymes, and these results may contribute to the cutaneous antimicrobial barrier.

Poster Presentation : **LIFE.P-372**

Life Chemistry

Event Hall FRI 11:00~13:00

Inhibitory effect on inflammation and obesity aggravated by induction of high-fat diet of herbal extract mixture

Seung yu Choi, In-Ah Lee[1,*]

Chemistry, Kunsan National University, Korea

[1]*Department of Chemistry, Kunsan National University, Korea*

Cnidium Officinale, *Paeonia japonica*, and *Angelica Gigas Nakai* well known as herbal medicines have been recognized for their efficacy and are being used as materials for various health-improving foods and over-the-counter medicines.In this study, the effect of synergistic effect on obesity by mixing lactobacillus in *Cnidium Officinale* water extract, *Paeonia japonica* water extract, *Angelica Gigas Nakai* water extract.To confirm the anti-obesity effect, obesity was induced by eating a high-fat diet in mice, and the prepared sample was administered every day for 8 weeks.As a result of checking various indices that can confirm obesity through biochemical analyzers, it was confirmed that when lactobacillus was mixed with *Cnidium Officinale* water extract, *Paeonia japonica* water extract, and *Angelica Gigas Nakai* water extract respectively, it showed a tendency to suppress obesity.In addition, amino acids with the highest content were identified through amino acid analysis, and the degree of change in intestinal bacteria was confirmed through analysis of mouse feces.

Poster Presentation : **LIFE.P-373**

Life Chemistry

Event Hall FRI 11:00~13:00

The effect of improving obesity and suppressing inflammation in high-fat mice of *Inonotus Obliquus*, including glucose precipitate

Hyunsoo Kim, In-Ah Lee[1,*]

Chemistry department, Kunsan National University, Korea
[1]*Department of Chemistry, Kunsan National University, Korea*

Chaga mushrooms(*Inonotus Obliquus*) are medicinal mushrooms that have been used for centuries and are known to have excellent anticancer effects by many researchers.This study aims to prove the usefulness of improving obesity using Chaga mushrooms. The high-fat diet was fed to mice using *Inonotus Obliquus* water extract(IO), and IO glucose precipitate(IOP) was performed to confirm changes in body and lipid content and anti-inflammation efficacy. We would like to prove the usefulness of improving obesity using Chaga mushrooms. Obesity breaks the balance of the body and is accompanied by inflammation. *Inonotus Obliquus*, which are effective in cancer, were effective in inflammation. In particular, it was confirmed that obesity indicators were suppressed as a result of confirming the effect of obesity improvement through animal experiments using IO and IOP. The concentration of triglycerides in liver tissue decreased significantly as the *Inonotus Obliquus* water extraction experimental group and the IO glucose precipitate experimental group (IO, IOP) decreased 26.8%, 30.9%, and the total cholesterol decreased 61.9%, respectively. In addition, the composition of *Inonotus Obliquus* was identified using an amino acid analyzer, and additional components were identified through SOD-like activity, PCR, Western blot, and biochemical element analysis.

Poster Presentation : **LIFE.P-374**

Life Chemistry

Event Hall FRI 11:00~13:00

Abalone (*Haliotis discus*), identified different mechanisms for antibacterial and immune action of antimicrobial peptide isomers Ab2-5 and dAb2-5 purified from hdMolluscidin

Soo-cheol Choi, In-Ah Lee*

Department of Chemistry, Kunsan National University, Korea

Abalone-derived antibacterial peptides Ab2-5 and dAb2-5 which are preserved components of the innate immune system of all organisms were inductively formed by selecting where they represent the α-helix structure located in the center of hdMolluscidin. Ab2-5 and dAb2-5 are peptides whose C-terminus is amidated through the addition, substitution, and removal of amino acids, and are composed of 10 amino acids and have a low molecular weight of 1.5 kDa or less, and are rapidly absorbed in the body and have almost no side effects. also It has the strength of having strong physiological activity even with a small concentration. In this study, we tried to elucidate the mechanism of antibacterial, antioxidant, and anti-inflammatory immune activity of abalone-derived antibacterial peptides Ab2-5 and dAb2-5. In the case of antibacterial activity of Ab2-5 and dAb2-5, it has more positive charges than conventional antibacterial peptides, confirming that it has strong antibacterial power in both gram-positive bacteria(*C.albicans*), negative bacteria(*E.coli D31*), and fungi(*B.subtilis*) due to strong ion interaction. In addition, in the case of antioxidant and anti-inflammatory actions, it was found that both Ab2-5 and dAb2-5 blocked the binding between LPS-TLR4 receptors in LPS-induced RAW 264.7 cells due to strong binding to LPS. Meanwhile, in the case of dAb2-5, in addition to strong binding with LPS, it was confirmed through LPS-binding that there are other mechanisms for intracellular effects. From these results, it was confirmed that antibacterial peptides Ab2-5 and dAb2-5 were sufficiently usable as materials associated with antibacterial agents and anti-inflammation.

Poster Presentation : **ORGN.P-375**

Organic Chemistry

Event Hall FRI 11:00~13:00

Halogen Assisted Multiple Resonance Thermally Activated Delayed Fluorescence

Youngnam Lee, Jong-in Hong*

Department of Chemistry, Seoul National University, Korea

We have synthesized halogen-substituted multiple resonance (MR) thermally activated delayed fluorescence (TADF) emitters, namely, Cl-Mr and Br-MR. Cl-MR and Br-MR showed a decreased lifetime of delayed fluorescence and enhanced reverse intersystem crossing rate without any changes in ΔE_{ST} and orbital distribution compared to a non-halogenated MR emitter. As a result, Cl-MR showed a high photoluminescence quantum yield (PLQY) of 85% and an external quantum efficiency (EQE) of 27.2%. However, Br-MR didn’t have any enhancement in PLQY and EQE. Different performances of Cl-MR and Br-MR were rationalized by analyzing the rate constants of excited states and bond dissociation energies of carbon-halogen bonds.

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Poster Presentation : **ORGN.P-376**

Organic Chemistry

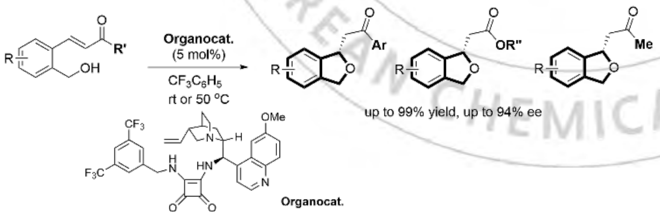
Event Hall FRI 11:00~13:00

Asymmetric organocatalytic intramolecular oxa-Michael reaction of α,β-unsaturated carbonyls containing benzyl alcohol

<u>Jae Eun No</u>, Seung Yeon Kim[1], Sung-Gon Kim[*]

Department of Chemistry, Kyonggi University, Korea
[1]*department of chemistry, Kyonggi University, Korea*

Organocatalytic enantioselective intramolecular oxa-Michael reactions of benzyl alcohol bearing α,β-unsaturated carbonyls as Michael acceptors are presented. Using cinchona squaramide-based organocatalyst, enones as well as α,β-unsaturated esters containing benzyl alcohol provided their corresponding 1,3-dihydroisobenzofuranyl-1-methylene ketones and 1,3-dihydroisobenzofuranyl-1-methylene esters in excellent yields with high enantioselectivities. In addition, enantioenriched 1,3-dihydroisobenzofuranyl-1-methylene ketone could be obtained from the Wittig/oxa-Michael reaction cascade of 1,3-dihydro-2-benzofuran-1-ol.



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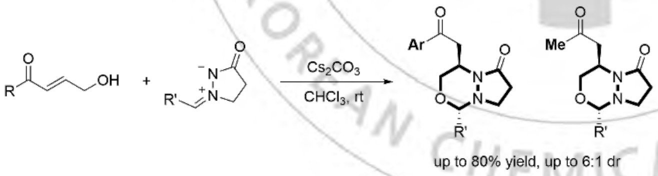
Poster Presentation : **ORGN.P-377**
Organic Chemistry
Event Hall FRI 11:00~13:00

Catalyst-free [3+3]-cycloaddition of γ-hydroxy-α,β-unsaturaded carbonyls and *N,N'*-cyclic azomethine imines

Sung Hyun Kang, ByungJun Park[1], Sung-Gon Kim[2,*]

Department of chemistry, Kyonggi University, Korea
[1]*department of chemistry, Kyonggi University, Korea*
[2]*Department of Chemistry, Kyonggi University, Korea*

The [3+3] cycloaddition reaction of various γ-hydroxy-α,β-unsaturaded carbonyls of *N,N'*-cyclic azomethine imines is presented. This cycloaddition reaction provides an attractive method for the synthesis of pyrazoloxadiazinone derivatives, which were obtained in good yields (up to 80% yield) and stereoselectivities (up to 6:1 dr). Moreover, the asymmetric cycloaddition reaction to furnish enantioenriched pyrazoloxadiazinones has also been established.



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Poster Presentation : **ORGN.P-378**

Organic Chemistry

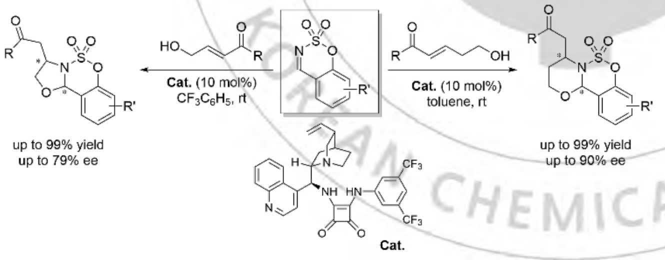
Event Hall FRI 11:00~13:00

Organocatalytic enantioselective cycloadditions of γ-hydroxy- and δ-hydroxy-α,β-unsaturaded carbonyls and cyclic *N*-sulfimines

Seung Yeon Kim, **Yoseop Kim**[1], **Sung-Gon Kim**[1,*]

department of chemistry, Kyonggi University, Korea
[1]*Department of Chemistry, Kyonggi University, Korea*

The first organocatalytic asymmetric [3+2]-cycloaddition of γ-hydroxy-α,β-unsaturated carbonyls with cyclic *N*-sulfimines is presented. This asymmetric reaction provided enantioenriched polyheterotricyclic 1,3-oxazolidines in high yields and with good enantioselectivities. This approach was also extended to the asymmetric [4+2]-cycloaddition of δ-hydroxy α,β-unsaturated carbonyls, affording enenatioenriched 1,3-oxazinanes in one step under mild conditions.



Poster Presentation : **ORGN.P-379**

Organic Chemistry

Event Hall FRI 11:00~13:00

Direct Cross-Coupling of Chiral Amino Acid Chlorides and Hydrocarbons Enabled by Mechanistically Controlled Nickel/Photoredox Dual Catalysis

Beomsoon Park, **Soon Hyeok Hong***

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The direct modification of naturally occurring chiral amino acids to their amino ketone analogs is a significant challenge in synthesis. Here, an efficient and robust cross-coupling reaction between chiral amino acid chlorides and unactivated C(sp^3)–H hydrocarbons was achieved by a mechanistically designed Ni/Ir photoredox catalysis. The reaction enabled unprecedented modular access to a wide variety of chiral amino ketones under mild reaction conditions with retention of the stereochemistry of the starting chiral amino acids. In-depth mechanistic analysis revealed that the strategical generation of an N-acyllutidinium intermediate is the key to success. The barrierless reduction of the N-acyllutidinium intermediate facilitates the reaction to deliver chiral amino ketones with retention of stereochemistry, bypassing the formation of a detrimental nickel intermediate which could be responsible for unwanted decarbonylation and transmetalation reactions majorly occurring in the previously reported methods.

Poster Presentation : **ORGN.P-380**
Organic Chemistry
Event Hall FRI 11:00~13:00

Development of Chemically Recyclable Polymers via Ring-Opening Metathesis Polymerization Using Rationally Designed Monomers

Kyungmin Choi, Soon Hyeok Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The development of chemically recyclable polymers is a pertinent challenge for a sustainable future The present study elaborately designed low-strained monomers to produce novel chemically recyclable polymers by ring-opening metathesis polymerization (ROMP). Density functional theory was used to predict the low-strained monomer reactivity by comparing their enthalpy change in ethenolysis reaction which is defined as ethenolysis ring strain energy. The ethenolysis ring strain energies could be modulated to allow highly efficient and controlled ROMP of the low-strained monomers. Open-loop recycling, as well as close-loop recycling, could be achieved by applying elaborately designed chemical transformations.

Poster Presentation : **ORGN.P-381**
Organic Chemistry
Event Hall FRI 11:00~13:00

Ring-Opening Metathesis Polymerization of 3-Acyloxycyclopentene: Control of Regioregularity and Dispersity

Jiyoung Lee, Soon Hyeok Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Ring-opening metathesis polymerization (ROMP) of low strain monomers is challenging due to the equilibrium between polymerization and ring-closing metathesis (RCM) depolymerization as well as possible chain transfer reactions. To overcome these limitations, ROMP of 3-acyloxycyclopentenes (3ROCOCPEs) with low ring strain energies (e.g., 3-acetoxycyclopentene (3AcCPE), RSE ~ 4.83 kcal/mol) was investigated by changing the steric bulkiness of the R substituent. The polymers having high regioregularity and narrow dispersity could be obtained by using sterically bulky 3ROCOCPE monomers with a trifluoromethanesulfonamide-based ruthenium catalyst at low temperatures. Regioselectivity, caused by the distal and proximal approach modes of the ruthenium catalyst to the monomer, was also controlled. The distal approach is generally preferred due to the steric repulsion of substituents, resulting in higher head-to-tail insertions. In addition, the chain transfer reaction could be suppressed by performing the ROMP with relatively bulky monomers under low-temperature conditions, producing polymers with narrow polydispersities.

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Poster Presentation : **ORGN.P-382**
Organic Chemistry
Event Hall FRI 11:00~13:00

Three-Component Decarboxylative Addition for the Synthesis of Vinyl Sulfones

An Seunghwan, Haeun Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

The $CuBr_2$/1,10-phenanthroline catalytic system in the presence of acetic acid provides the desired vinyl sulfones in moderate to good yield

Poster Presentation : **ORGN.P-383**

Organic Chemistry

Event Hall FRI 11:00~13:00

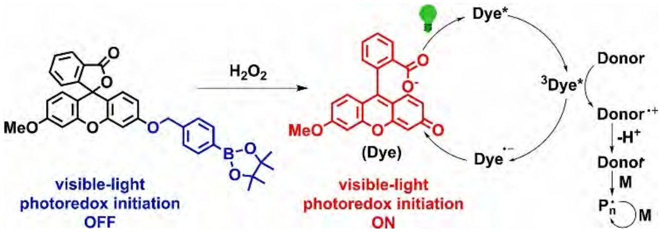
Photoinduced radical polymerization by methyl fluoresceins under visible light and the application to signal amplification of hydrogen peroxide

Joseph Nganga, Hyebin Ko, Won Oh Choi, Jungkyu K. Lee[1,*]

Chemistry, Kyungpook National University, Korea

[1]Department of Chemistry, Kyungpook National University, Korea

We investigated the relationship between the structure and photoredox catalytic performance of fluorescein in free-radical polymerization under visible light. Methyl fluorescein derivatives (methyl ether of fluorescein, methyl ester of fluorescein, and methyl ether ester of fluorescein) were synthesized and their photoredox catalytic performances, compared to that of fluorescein, were carefully analyzed. The mechanism of photoinduced electron transfer (PET) between each dye and triethanolamine was studied using Electron paramagnetic Resonance (EPR), Linear sweep voltammetry (LSV) and Steady-state Photolysis. As an application of our approach, we designed methyl ether of fluorescein bearing a boronate moiety as a H2O2-selective photoredox catalyst, to amplify the signal of H2O2 via photoinduced radical polymerization. Based on the results, methyl ether derivatives showed lower photoredox catalytic efficiency compared to those of fluorescein and methyl ester fluorescein. Restriction of tautomerization, caused by methylation of phenolic hydroxyl, is rationalized to be the main reason of the reduced efficiency. As for the sensing of H2O2 , the signal of hydrogen peroxide (down to 20 μM) was successfully detected by 10 μM of the photoredox catalyst. We hope that the results highlighted in this research would contribute to the design of new fluorescein-based photoredox catalysts and probes, with potential applications in polymer chemistry, organic synthesis, and medical-related sciences.



Poster Presentation : **ORGN.P-384**

Organic Chemistry

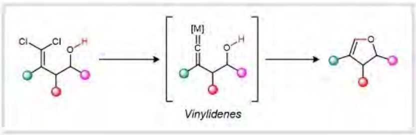
Event Hall FRI 11:00~13:00

Catalytic Reductive Vinylidene Transfer via 1,5-O－H bond Insertions

Houng Kang

Department of Chemistry Education, Chungbuk Natioanl University, Korea

Vinylidenes have been attention as reactive intermediates for organic transformations. The vinylidene are known to activate a various type of bonds, such as C-H, O-H, N-H, and O-Si bonds, owing to their electronic property. Contrasting to intramolecular 1,5-C-H bond insertions, however, only few examples of intramolecular polarized bond insertions have been reported due to their harsh conditions as well as the competing 1,2-migration process, Fritsch-Buttenberg-Wiechell rearrangement, in conventional free vinylidene methods. Here, we demonstrated nickel-catalyzed vinylidene transfer reaction by means of an intramolecular 1,5-O-H insertions. Our approaches to generate alkylidenecarbenes from 1,1'-dichloroalkene, which can be prepared from aldehydes or ketones, allowed access to 2,3-dihydrofurans under nonbasic conditions.



Poster Presentation : **ORGN.P-385**

Organic Chemistry

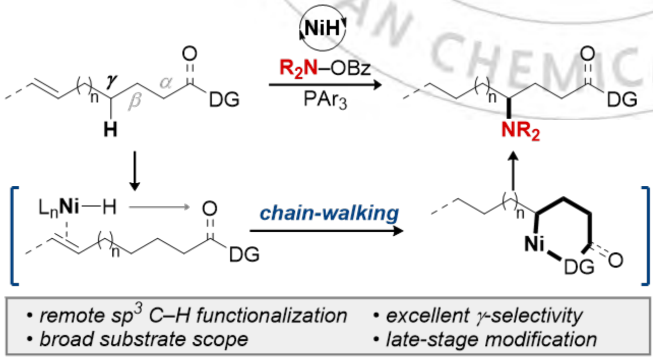
Event Hall FRI 11:00~13:00

γ-Selective Migratory Amination via Controlled Chain Walking Strategy

Changseok Lee, **Sungwoo Hong**[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Regioselective migratory functionalization through chain walking strategy has attracted considerable attention as a powerful tool to achieve selective C(sp3)–H functionalization in the presence of multiple similar aliphatic C–H bonds. Despite the significant efforts in this field, migratory functionalization reactions are limited to C(sp3)–H α and β to polar-functional units, while γ-C(sp3)–H functionalization through controlled alkene transposition is a longstanding challenge. Herein, we represent γ-selective migratory amination through Ni catalyzed alkene isomerization by external phosphine ligand and thermodynamically stable 8-aminoquinoline (AQ)-chelated nickellacyle, subsequently interrupted by an aminating reagent. Moreover, unusual δ-selective amination was developed by employing picolinamide (PA)-tethered alkene substrates to afford synthetically challenging and important chemical building blocks.



129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-386**

Organic Chemistry

Event Hall FRI 11:00~13:00

ATP sensing and imaging nanoprobe based on AIEgen in cancer and embryonic stem cells

Byeong Wook Kim, Dokyoung Kim[1,*], Byeong Moon Kim[2,*]

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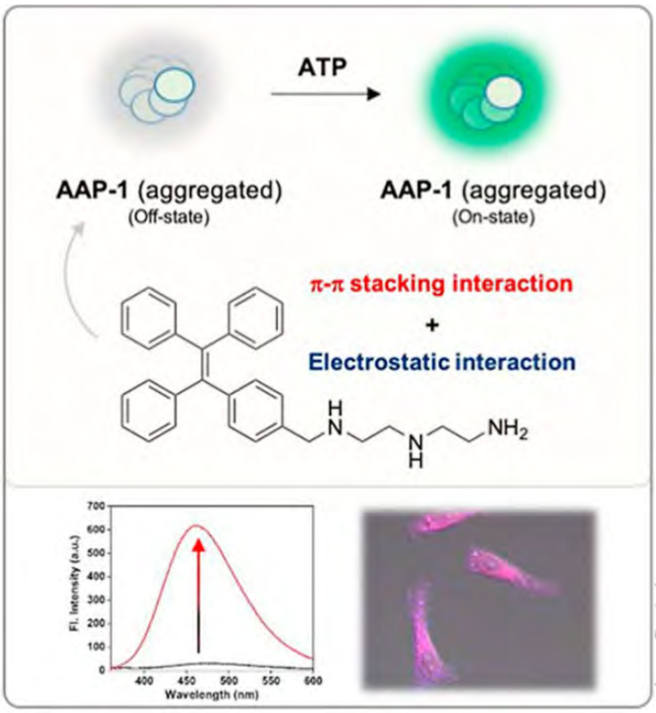
[1]*College of Medicine, Kyung Hee University, Korea*
[2]*Division of Chemistry, Seoul National University, Korea*

ATP is a biological molecule that plays essential roles in cells such as the primary carrier of energy, intracellular signaling, amino acid activation in protein synthesis, immune response, DNA/RNA synthesis, and growth. Because of its importance, analytical methods to monitor ATP have been developed. Among them, a small organic fluorescence probe for the ATP has received attention because of their ease-of-use and wide range of application.We disclose herein a new turn-on fluorescent nanoprobe (named AAP-1), based on an aggregation-induced emission luminogen (AIEgen). The organic fluorophore (named TPE-TA) is composed of tetraphenylethylene (TPE, sensing and signaling moiety) and triamine (TA, sensing moiety). In aqueous media, TPE-TA turns to an aggregated form as a nanoprobe AAP-1 and shows electrostatic and hydrophobic interactions with ATP simultaneously. The AAP-1 displays excellent selectivity toward ATP, reliable sensitivity (0.275 ppb), and fast signal response (


ATP
AAP-1 (aggregated)
(Off-state)
AAP-1 (aggregated)
(On-state)
π-π stacking interaction
+
Electrostatic interaction
H
N
N
H
NH2
Fl. Intensity (a.u.)
700
600
500
400
300
200
100
0
400
450
500
550
600
Wavelength (nm)

Poster Presentation : **ORGN.P-387**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Mollugin Derivatives

Yong-Suk Jang, Nam-Jin Chung[1], Beom-tae Kim[2,*]

Division of Life Sciences Molecular Biology Major, Reserch Center of Bioactive Materials, Korea
[1]*Department of Crop Science and Biotechnology, Reserch Center of Bioactive Materials, Korea*
[2]*Department of Bioenvironmental Chemistry, Reserch Center of Bioactive Materials, Korea*

Mollugin has been used as a herbal medicine for anti-arthritis, anti-dysmenorrhea, hemostasis from the past. It was extracted from the medicinal plant, Rubia cordifolia in China and India.In the recent study, mollugin has been reported to show new biological properties such as anti-tumor, anti-mutagenic, anti-leukemia, anti-inflammatory, and anti-allergic activities.Despite reports on the various pharmacological effects of molligin, the synthetic efforts to prepare derivatives and thereby the estimation on the structure-activity relationship have not been examined. As the primary work, we attempted to synthesize mollugin derivatives in which benzene moiety of mollugin is mono- or di-substituted with methoxy groups. Diverse synthetic methodologies have been tried to prepare mollugin derivatives and would be presented here.

Poster Presentation : **ORGN.P-388**
Organic Chemistry
Event Hall FRI 11:00~13:00

Genetic encoding of fluorogenic synthetic amino acids for bioimaging

Hwiyeong Lee, Minseob Koh*

Department of Chemistry, Pusan National University, Korea

Genetically encoded fluorescent proteins have been used to visualize a large variety of proteins and investigate their biological processes. Despite the versatile use of green fluorescent protein (GFP) derivatives, size (> 20 kDa) and the requirement of terminal site fusion limit their utility. To address this issue, we will develop a genetically encoded fluorogenic amino acid (fAA) for bioimaging application. The genetic code expansion strategy enabled site-specific incorporation of a synthetic noncanonical amino acid to the protein, so that structural perturbation of the target protein is minimal. We are using an arylideneimidazolinone as a core by mimicking GFP fluorophore 4-hydroxybenzlidene imidazolinone. We will construct a series of arylideneimidazolinonyl (homo)alanine (termed AIA) to generate fAAs in full-visible color range. As the first step on a long journey, we have synthesized a 4-(benzylidene)-1-aminopropanoic acid-2-methyl-5-imidazolinone (termed AIA-1). An oxazolone was synthesized by aldol condensation between *N*-acetylglycine and benzaldehyde with moderate yield (yield: 60%). Following hydrolysis provided a carboxylic acid with a good yield (yield: 90%), which was reacted with 2-(*S*)-(*tert*-butoxycarbonylamino)-3-aminopropionic acid by amide coupling under condition with EDC/DIPEA/HOBt (yield: 94%). Next step was the cyclization to generate imidazolinone by DBU condition (yield: 66%). The final product was obtained by treating a trifluoroacetic acid for *t*-BOC deprotection (yield: quantitative). We confirmed that the AIA-1 can be passed through cell wall of *E. coli* and present until 24 h in the cytosol by the mass spectrometry analysis. The AIA-1 exhibited fluorescent properties (emission maximum: 493 nm and 588 nm) in the viscous solvent (glycerol), whereas the intensity in water was dropped c.a. 5-fold. To encode the AIA-1 to the target genes in *E. coli*, we are now constructing a *M. barkeri* pyrrolysyl-tRNA synthetase library by site-saturation mutagenesis at the amino acid binding sites (A267, L270, Y271, L274, C313, and W383). At the same time, we are expanding the AIA series that contain different substituent on the benzene ring to render electronic variation of the fluorophore. Once it is encoded, the small-size and full-color tunability of AIA series will be a powerful tool kit to study biomolecules.

Poster Presentation : **ORGN.P-389**

Organic Chemistry

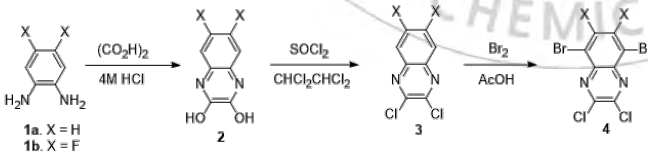
Event Hall FRI 11:00~13:00

A concise synthesis and optical properties of multi-halogenated quinoxaline derivatives

Kyukwan Zong*, **Hwanhee Jo**

Department of Chemistry Education, Jeonbuk National University, Korea

Multi-halogenated quinoxaline derivatives were synthesized through several steps starting from 1,2-diaminobenzene or 4,5-difluorobenzene-1,2-diamine. The condensation of 1,2-diaminobenzene or 4,5-difluorobenzene-1,2-diamine with oxalic acid under environmentally benign aqueous acidic condition afforded the corresponding quinoxlaine-2,3-diol (2) in good yield respectively. These diols were easily converted into the corresponding 2,3-dichloroquinoxaline (3) with treatment of thionyl chloride, which further functionalized into 5,8-dibromo-2,3-dichloroquinoxaline (4). Bromination of 2 also gave the corresponding 5,8-dibromoquinoxaline. These simple and high yielding procedures toward multi-halogenated quinoxaline derivatives are very useful for synthesis of D-A conjugated polymers for organic solar cells. The study also described further functionalization of 2 and selective coupling reactions of 4 for useful donor units.



129th General Meeting of the Korean Chemical Society
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Poster Presentation : **ORGN.P-390**

Organic Chemistry

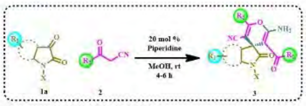
Event Hall FRI 11:00~13:00

Synthetic Annulation of Spiro Indoline-3, 4’-Pyran Based on Active Carbonyl Compounds with 1-Cyanoketones

Maruti Yadav, Yeon Tae Jeong*, Hoon Heo, Byung-Gwon Cho

Department of Display Engineering, Pukyong National University, Korea

A novel and efficient method for the construction of spiro indoline-3, 4’-pyran compound from 1-cyanoketones and 1, 2-diketone has been developed. The synthesis proceeded through the Knoevenagel, Michael adduct via intramolecular/Paal-Knorr cyclization under similar reaction condition. The less commonly used 1-cyanoketones and active carbonyl compounds served as the indole containing pyran source for the preparation of series of heterocyclic compounds. This heterocyclic structure allows one tetra-substituted carbon center and sequential hexa cyclic core under very mild conditions and shows excellent chemo and regioselectivity.



Poster Presentation : **ORGN.P-391**

Organic Chemistry

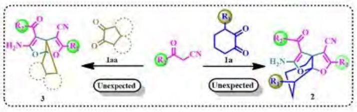
Event Hall FRI 11:00~13:00

DBU-Promoted Knoevenagel, Michael via Intramolecular/Paal-Knorr Cyclization of Novel Heterocyclic [3.3.3] and [4.3.3] Propellanes from α-Cyanoketones and cyclic α-Diketones.

<u>Maruti Yadav</u>, Yeon Tae Jeong*, Hoon Heo, Byung-Gwon Cho

Department of Display Engineering, Pukyong National University, Korea

An effective base-catalyzed Knoevenagel, Michael and intramolecular/Paal-Knorr cyclization strategy for the construction of heterocyclic [4.3.3] tetrahydro epoxyetheno benzo-furan propellanes (TEBFs) and fused epoxyetheno indeno [1, 2-b] furan [3.3.3] propellanes (EIFs) from cyclic α-diketones and α-cyanoketones is reported through single-step reaction. The reaction proceeds under mild reaction conditions in the absence of any external transition metal and ligands. The one-pot two-component procedure also shows the merits of straightforward reaction conditions, simple operation, using available feed-stock, wide substrate scope, and high atom and step economy. This reaction provides facile access to highly substituted fused tetrahydro furo-furan propellanes, which can be used in the field of chemical and pharmaceutical research.



Poster Presentation : **ORGN.P-392**

Organic Chemistry

Event Hall FRI 11:00~13:00

Renewable Catalytic Transformation of Carbohydrates to 2,5-Diformylfuran

Kihyuk Sung, Hye-Young Jang[1,*]

Department of Energy Systems Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

Lignocellulosic biomass, the most abundant carbon source, is expected to play an important role in the production of high-value chemicals and fuels through catalysis. C5 and C6 sugars from nature can be converted to furan molecules such as 5-hydroxymethylfuran (HMF) and 2,5-diformylfuran (DFF). DFF has potential applications as a monomer of polymers, heterocyclic ligands, luminophores, and platform chemicals. Many synthetic protocols of DFF from fructose were reported recently. However, these methods involve high temperature (150 ^{o}C) or several steps: dehydration of fructose to HMF with Brønsted acid, and generation of DFF through the oxidation of HMF. We report the one-step homogeneous approach transforming various carbohydrates to DFF with high yields under mild conditions. Furthermore, we successfully examined a heterogeneous system for the recyclability of the catalytic system.

Poster Presentation : **ORGN.P-393**

Organic Chemistry

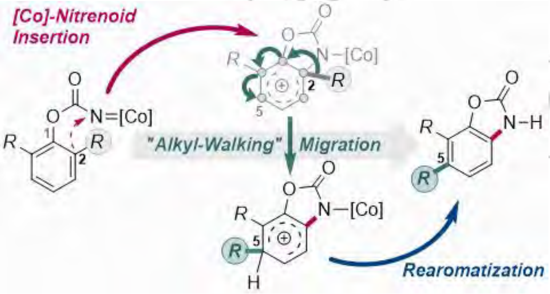
Event Hall FRI 11:00~13:00

Cobalt−Nitrenoid Insertion-Mediated Amidative Carbon Rearrangement via Alkyl-Walking on Arenes

Jeonghyo Lee, Sukbok Chang*

Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea

This work demonstrated the Cp*Co(III)(LX)-catalyzed amidative alkyl migration using 2,6-disubstituted phenyl azidoformates. Upon the cobalt−nitrenoid insertion toward the substituted ortho carbon, an arenium cationic species bearing a quaternary carbon is generated, and a subsequent alkyl migration process is suggested to occur through an unforeseen alkyl-walking mechanism. A quinolinol ligand of the cobalt catalyst system is proposed to facilitate the final product-releasing rearomatization process by serving as an internal base. This new mechanistic mode enabled both [1,2]- and [1,4]-alkyl rearrangements to allow the structural variation of N-heterocyclic compounds.



Poster Presentation : **ORGN.P-394**
Organic Chemistry
Event Hall FRI 11:00~13:00

KO*t*Bu-Catalyzed 1,2-Silaboration of N-Heteroarenes to Access 2-Silylheterocycles: A Cooperative Model for the Regioselectivity

Eunchan Jeong, Joon Heo, Dongwook Kim[1], Sukbok Chang[2,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*
[2]*Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea*

Reductive functionalization of N-heteroarenes offers a route to highly versatile heterocyclic synthons bearing multiple transformable groups. We present herein the development of KO*t*Bu-catalyzed 1,2-silaboration of a broad range of N-heteroarenes under mild condition. The scope was found to be broad to include (iso)quinolines, pyridines, and additional heterotoarenes. This convenient procedure furnishes (N-boryl) cyclic allylamino or enamino skeletons with the simultaneous sp^3 C–Si bond formation, which could be readily isolated as N-acyl products. Rearomative treatment of the partially reduced labile compounds was proven to offer a route to 2-silyl-N-heteroarenes. A model of the 6-membered ion-pair complex was proposed to rationalize the observed 1,2-regioselectivity, wherein KO*t*Bu catalyst plays an associative role in activating the substrate and silylborane reagent.

Poster Presentation : **ORGN.P-395**

Organic Chemistry

Event Hall FRI 11:00~13:00

Pd nanoparticles on alkylated triazine COFs: Synthesis, characterization and catalytic activity

Hyun Woo Song, Jung Heum Shin[1], Minkyung Lim, Hakjune Rhee[1,*]

Department of Chemical and Molecular Engineering, Hanyang University, Korea
[1]*Department of Applied Chemistry, Hanyang University, Korea*

Palladium nanoparticles immobilized on alkylated terephthaloylamide COFs have been prepared. Utilizing electron rich nature of nitrogen in trazine, Pd nanoparticles were effectively stabilized. Hydrophobic nature of alkyl chains had accelerated reactivity in heterogeneous coupling reaction by adsorbing starting organic compounds. Moreover, increasing specific surface and pore volume from previous research, better performance in Suzuki-Miyaura coupling reaction was observed. Sonogashira coupling reaction optimization was also conducted to confirm its reactivity. Various characterization techniques such as XPS, ICP, SEM, TEM, 1H- and 13C- NMR are used to verify the efficiency of the catalyst.

Poster Presentation : **ORGN.P-396**

Organic Chemistry

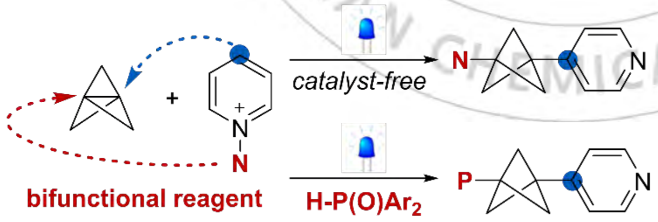
Event Hall FRI 11:00~13:00

Visible-Light-Induced Catalyst Free Pyridylation of [1.1.1]Propellane Using N-Aminopyridinium Salts

Sanghoon Shin, Sungwoo Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The visible-light-induced strain-release aminopyridiylation of propellanes has been developed by employing N-aminopyridinium salts as bifunctional reagents under extremely mild reaction conditions. This strategy involves the photoactive formation of N-aminopyridinium salts, which enables the direct incorporation of amino and pyridyl groups onto BCP frameworks without requiring a photocatalyst. The present procedure exhibits a fairly broad substrate scope and offers a convenient and powerful synthetic tool for accessing 1,3-aminopyridylated BCPs. Furthermore, this strategy can be extended to P- radicals, offering the option of divergence via the three-component assembly of valuable BCP chemical entities. Overall, this versatile method significantly expands the scope of BCP-type bioisosteres and is expected to stimulate further research endeavors for applications in medicinal chemistry.



Poster Presentation : **ORGN.P-397**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Electroluminescent Properties of 4-(10-phenylanthracen-9-yl)-9,9'-spirobi[fluorene] Derivatives for Blue Organic Light-Emitting Diodes

Jinyeong Heo, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

Continuous research and development of blue OLED materials are necessary to achieve their desired performance. In this study, three blue fluorescent materials based on the 9-substituted 10-phenylanthracene were synthesized and characterized for organic light-emitting diodes (OLEDs). Their photophysical properties, molecular configurations and electroluminescent properties have been investigated. To study their electroluminescent properties, the OLEDs devices were fabricated in the following sequence: indium-tin-oxide (ITO, 180 nm) / 4,4'-bis(N-(1-naphthyl)-N-phenylamino) biphenyl (NPB, 50 nm) / blue fluorescent materials (20 nm) / bathophenanthroline (Bphen, 30 nm) / lithium quinolate (Liq, 2 nm) / Al (100 nm). Particularly, a device using 4'-(10-phenylanthracen-9-yl)spiro[benzo[b]fluoreno[3,4-d] thiophene-7,9'-fluorene] in emitting layer exhibits the maximum external quantum efficiency (EQE) of 3.20% with Commission International de L'Eclairage (CIE) coordinates of (0.15, 0.13) at 6.0 V.

Poster Presentation : **ORGN.P-398**

Organic Chemistry

Event Hall FRI 11:00~13:00

Glucose Oxidase-Mediated Oxidation of Fe^{2+}-Tannic Acid Complex for Catalytic Single-Cell Nanoencapsulation

Duc Tai Nguyen, Hojae Lee, Nayoung Kim, Insung Choi[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Single-cell nanoencapsulation (SCNE) aims to construct cell-in-shell biohybrid structures, where individual cells are encased with nanometric sheaths. The shells are required to be cytoprotective, and preferably, endow the cells with exogenous functions. Correspondingly, methodological development for the construction of catalytically functional shells has been an intense research topic in SCNE. This work proposes a one-step approach to synthesis of enzyme-embedded artificial shells that encapsulate individual *Saccharomyces cerevisiae*. Specifically, hydrogen peroxide, generated by the enzymatic reaction of glucose oxidase with glucose, facilitates the oxidation of Fe^{2+} to Fe^{3+} in the Fe^{2+}-tannic acid complex and the construction of Fe^{3+}-tannic acid shells on individual living cells, as well as the concomitant embedment of glucose oxidase with sustained catalytic activity. This method provides a facile bioaugmentation strategy for empowering living cells with exogenous functions.

Poster Presentation : **ORGN.P-399**

Organic Chemistry

Event Hall FRI 11:00~13:00

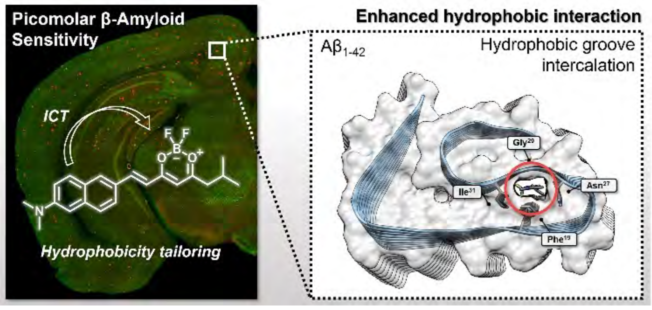
Tailoring the Hydrophobicity of Small-Molecular Fluorophores toward Picomolar-Sensitive Optical Imaging of Amyloid Beta in Alzheimer's Disease

Jusung An, Peter Verwilst[1], Jinwoo Shin, Ilwha Kim, Jongseung Kim[*]

Department of Chemistry, Korea University, Korea

[1]*Department of Medicinal Chemistry, Rega Institute for Medical Research, Belgium*

The pathological origin of Alzheimer's disease (AD) is still shrouded in mystery. The selective visualization of amyloid beta (Aβ), the most abundant proteinaceous deposit, is pivotal to revealing AD pathology. Unlike enzymes or receptors with specific binding sites, Aβ is an atypical protein exhibiting less predictable binding modes with small-molecular ligands. The Aβ has the structural characteristic "cross-β-sheet" scaffold, in which adjacent chain segments are tightly folded in an anti-parallel way within the fiber lattice. Based on the intrinsic hydrophobicity of Aβ, small molecule dyes have been postulated to bind *via* hydrophobic π-π stacking interactions to these β-sheets surfaces or intercalate into hydrophobic grooves and channels.To date, several small-molecule fluorophores for Aβ have been developed with increasing binding affinities through enhancing hydrophobicity. However, the increased hydrophobicity associated with an extended π-conjugation inevitably leads to poor aqueous solubility and induces the ligands' promiscuity regarding other hydrophobic proteins and cellular components. Thus, the major challenge in designing new red-emissive dyes with a stronger affinity for Aβ fibrils is maintaining adequate aqueous solubility specificity, and sensitivity.In this work, small-molecular dioxaborine-derived dyes were rationally designed by tailoring the hydrophobicity to enhance the binding affinity for $A\beta_{1-42}$ fibrils —while concurrently preventing poor aqueous solubility—*via* biannulate donor motifs in D-π-A dyes. An unprecedented sub-nanomolar affinity was found ($K_d = 0.62 \pm 0.33$ nM) and applied to super-sensitive and red-emissive fluorescent staining of amyloid plaques in cortical brain tissue *ex vivo*.


Picomolar β-Amyloid Sensitivity
ICT
Hydrophobicity tailoring
Enhanced hydrophobic interaction
Aβ1-42
Hydrophobic groove intercalation
Gly20
Ile31
Asn27
Phe19

Poster Presentation : **ORGN.P-400**

Organic Chemistry

Event Hall FRI 11:00~13:00

Asymmetric Total Syntheses of (+)-Decursivine and (+)-Serotobenine via Intramolecular Fischer Indole Synthesis

Hyo-Mi Kim, Hyunwoo Lee, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

We have previously demonstrated that aryl hydrazide with a carbonyl function linked to meta- or para-position through an appropriate tether may undergo a Fischer-type indolization to afford 3,4- or 3,5-fused tricyclic indole.[1] Such intramolecular Fischer indole synthesis (IMFIS) proved effective in the synthesis of 3,4-fused tricyclic indole natural product (+)-aurantioclavine.[1a)] As a part of our ongoing campaign on the IMFIS strategy toward target-oriented synthesis, we have proposed a new asymmetric synthetic approach to (+)-decursivine and (+)-serotobenine. The highlights are the intramolecular Fischer indolization of aryl hydrazide for the de novo construction of the critical 8-membered 3,4-fused tricyclic indole ring system, and the Rh-carbenoid mediated enantioselective intramolecular asymmetric C-H insertion reaction of α–diazo lactam for the stereocontrolled assembly of the dihydrobenzofuran unit.[2] BF_3 etherate-mediated epimerization and deprotection of the two nitrogen masking groups culminated in the asymmetric total syntheses of the targeted natural compounds.**References**1. a) Park, J.; Kim, D.-H.; Das, T.; Cho, C.-G. *Org. Lett.* **2016**, *18*, 5098-5101. b) Park, J.; Kim, S.-Y.; Kim, J.-E.; Cho, C.-G. *Org. Lett.* **2014**, *16*, 178-181.c) Park, I.-K.; Park, J.; Cho, C.-G. *Angew. Chem. Int. Ed.* **2012**, *51*, 2496-2499. 2.a) Santiago, V.; Machado, A. H. L. *Beilstein J. Org. Chem.* **2016**, *12*, 882-902. b) Doyle, M. P.; Duffy, R.; Ratnikov, M.; Zhou, L. *Chem. Rev.* **2010**, *110*, 704-724. c) Davies, H. M. L.; Denton, J. R. *Chem. Soc. Rev.* **2009**, *38*, 3061-3071. d) Davies, H. M. L.; Manning, J. R. *Nature* **2008**, *451*, 417-424. e) Robinson, E. E.; Thomson, R. J. *J. Am. Chem. Soc.* **2018**, *140*, 1956-1965.

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Poster Presentation : **ORGN.P-401**

Organic Chemistry

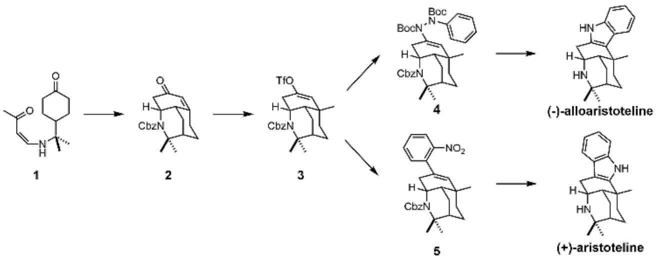
Event Hall FRI 11:00~13:00

Total Syntheses of Aristotelia Alkaloids

<u>Tae-Hong Jeon</u>, Cheon-Gyu Cho*

Department of Chemistry, Hanyang University, Korea

Abstract We have previously demonstrated that ene-hydrazides prepared from enol triflates in regiochemically defined form may undergo Fischer indolization reactions without regiochemical scrambling.[1] This synthetic strategy has been successfully applied to the total synthesis of (+)-aspidospermidine, (-)-tabersonine, (+)-uleine, and (-)-tubifolidine.[2] As a part of our ongoing study for applying this method to the synthesis of natural products, we designed new synthetic routes toward the total syntheses of *aristotelia* alkaloids, (-)-alloaristoteline and (+)-aristoteline. We began the synthetic exploration by furnishing the critical tricyclic core via the intramolecular Robinson annulation process from enone **1**. Subsequent 1,4-addition followed by *in-situ* triflation afforded the enol triflate **3**. Palladium-catalyzed C-N coupling of enol triflate with phenyl hydrazide and indolization under Lewis acidic condition led to the total synthesis of (-)-alloaristoteline. Alternatively, by Suzuki coupling, *o*-nitrostyrene **5** could be prepared from enol triflate and subsequent reductive cyclization afforded (+)-aristoteline. Presented herein are the total syntheses of (-)-alloaristoteline and (+)-aristoteline.**References**1.(a) Kim, J.-Y.; Lee, W.; Kang, H.-J.; Jeon, T.-H.; Baik, M.-H.; Cho, C.-G. *ACS Catal.*, **2021**, *11*, 12821.(b) Lim, B.-Y.; Jung, B.-E.; Cho, C.-G. *Org. Lett.*, **2014**, *16*, 4492.2.(a) Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett.*, **2017**, *19*, 6168.(b) Kim, D.-H.; Kim, J.-H.; Jeon, T.-H.; Cho, C.-G. *Org. Lett.* **2020**, *22*, 3464.



Poster Presentation : **ORGN.P-402**

Organic Chemistry

Event Hall FRI 11:00~13:00

A new approach to the synthesis of (+)-limaspermidine

Sang-Ha Oh, **Cheon-Gyu Cho***

Department of Chemistry, Hanyang University, Korea

We have investigated 3,5-dibromo-2-pyrone towards target-oriented synthesis, utilizing its peculiar reactivity as a neutral diene as well as the selective maneuverability of the two bromine groups. Such efforts have resulted in successful syntheses of an array of biologically important natural products.[1] Inspired by our previous results, we elaborately devised a new synthetic route to (+)-limaspermidine. In order to confer the required chirality to the synthesis, the bicyclolactone prepared from the Diels-Alder reaction of 3-phenyl-5-bromo-2-pyrone was resolved into its enantiomers using quinidine as a chiral base.[2] Subsequent transformations, including intramolecular Pd-catalyzed aromatic C-H amination[3] to construct the key indolenine subunit, allowed us to complete the asymmetric formal total synthesis of (+)-limaspermidine.**References**1.(a) Kim, W.-S.; Kim, H.-J.; Cho, C.-G. *J. Am. Chem. Soc.* **2003**, *125*, 14288. (b) Tam. N. T.; Cho, C.-G. *Org. Lett.* **2007**, *9*, 3391. (c) Shin, I.-J.; Choi, E.-S.; Cho, C.-G. *Angew. Chem. Int. Ed.* **2007**, *46*, 2303. (d) Chang, J. H.; Kang, H.-U.; Jung, I.-H.; Cho, C.-G. *Org. Lett.* **2010**, *12*, 2016. (e) Jung, Y.-G.; Kang, H.-U.; Cho, H.-K.; Cho, C.-G. *Org. Lett.* **2011**, *13*, 5890. (f) Jung, Y.-G.; Lee, S.-C.; Cho, H.-K.; Nitin B. D.; Song, J.-Y.; Cho, C.-G. *Org. Lett.* **2013**, *15*, 132. 2.Jeon, T.-H.; Kang, H.-J.; Svirid, A.; Lyakhov, A.; Kovalenko, V; Cho, C.-G. *Bull. Korean Chem. Soc.* **2019**, *40*, 910.3. He, G.; Lu, C.; Zhao, Y.; Nack, W.-A.; Chen, G. *Org. Lett.* **2012**, *14*, 2944.

Poster Presentation : **ORGN.P-403**
Organic Chemistry
Event Hall FRI 11:00~13:00

Tandem C3-selective Stille Cross-Coupling/IMDA Cascade of 3,5-Dibromo-2-pyrones for the Asymmetric Total Syntheses of (+)-Lycopladine A and (-)-Lycoposerramine R

Thameem Ul Ansari, Sang-Ha Oh, Hyewon Min, Dayun Jeon, Hyunwoo Kim[1,*], Cheon-Gyu Cho[*]

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Lycopodium alkaloids are a structurally diverse class of natural products found in plants of the widely distributed Lydopodium genus, also known as club mosses, belonging to the plant family Lycopodiaceae.[1] They display various biological activities ranging from acetylcholine esterase inhibitory to antitumor properties. Lycopladine A, isolated from Lycopodium complanatum in 2006 by Kobayashi and co-workers,[2] has received the most attention for the synthesis.As a part of our ongoing exploration of 3,5-dibromo-2-pyrone toward target-oriented synthesis, we have proposed a novel synthetic route to (+)-lycopladine A and (-)-lycoposerramine R. In general, 2-Pyrones with a chiral branched allylic silyl ether undergoes IMDA reactions with remarkably and unprecedentedly high levels of π-facial- and endo-selectivity.[3]The resulting diastereomerically and enantiomerically pure cycloadducts were readily transformed into the natural products (+)-lycopladine A and (-)-lycoposerramine R. The key reactions in the total syntheses are intermolecular Stille coupling with pyridine stannane, Barton Macomb deoxygenation reaction, and regioselective hydroboration reaction.**Acknowledgments**This work was supported by the National Research Foundation of Korea.**References**1) For recent reviews, see: L. Rodrigues, M. S. Majik, *Asian J. Org. Chem.* **2019**, *8*, 1151-1163; a) M. Saha, R. G. Carter, *Synlett* **2017**, *28*, 2212-2229; b) R. A. Murphy, R. Sarpong, *Chem. Eur. J.* **2014**, *20*, 42-56; c) X. Wang, H. Li, X. Lei, *Synlett* **2013**, *24*, 1032-1043; d) P. Siengalewicz, J. Mulzer, U. Rinner in The Alkaloids: *Chemistry and Biology*, Vol. 72 (Ed.: K. Hans-Joachim), Academic Press, **2013**, pp. 1-151; e) A. Nakayama, M. Kitajima, H. Takayama, *Synlett* **2012**, *309*, 1-32; f) M. Kitajima, H. Takayama, Top. *Curr. Chem.* **2012**, *309*, 1-32; h) X. Ma, D. R. Gang, *Nat. Prod. Rep.* **2004**, *21*, 752-772; j) W. A. Ayer, *Nat. Prod. Rep.* **1991**, *8*, 455-463.

2) K. I. Ishiuchi, T. Kubota, H. Morita, J. I. Kobayashi, *Tetrahedron Lett.* **2006**, *47*, 3287-3289.3) J.-H. Lee, C.-G. Cho, *Org. Lett.* **2018**, *20*, 7312−7316.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-404**

Organic Chemistry

Event Hall FRI 11:00~13:00

Total Synthesis of Ervatamine

<u>Qinyang Chen</u>, Cheon-Gyu Cho[1,*]

chemistry, Hanyang University, China
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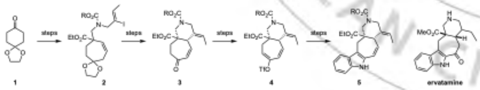
Abstract Ervatamine is a novel 2-acylindole alkaloid extracted from Ervatamia Orientalis through ethanol.[1] It has the cyclohepta[b]indole as the core structure, obtained from regioselective indolization. As a part of our ongoing study on regioselective Fischer Indole synthesis,[2] we have envisaged a new synthetic route to ervatamine. The bicyclic ring was furnished from alkene **3** via intramolecular Heck reaction. Copper-catalyzed C-N coupling of enol triflate with phenyl hydrazide and indolization under Lewis acidic conditions led up to ervatamine. Presented herein is our recent progress toward the total syntheses of ervatamie.**References**1.Knox, J R, Slobbe, J. *Aust. J. Chem.*, **1975**, *28*, 1813.2.(a) Lim, B.-Y,; Jung, B.-E,; Cho, C.-G. *Org. Lett*. **2014**, *16*, 4492.(b) Kim, J.-Y.; Suhl, C.-H.; Lee, J.-H.; Cho, C.-G. *Org. Lett*. **2017**, *19*, 6168.



Poster Presentation : **ORGN.P-405**

Organic Chemistry

Event Hall FRI 11:00~13:00

Catalyst-free α-C–H Amination of Cyclic Amine Scaffolds Enabled by Photo-Induced Polar-Radical Relay

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Aminals have been attractive targets in synthetic chemistry and medicinal field since they are widely present in biologically important molecules, such as alkaloid natural products as well as pharmaceutical drugs. As a result, the development of efficient and selective methods for generation of aminal moiety has been one of the major research topics. Recently, direct fucntionalization of a native C–H bond adjacent to nitrogen atom of amine has been emerged. It can offer a great opportunity to expand the practical synthetic routes to this aminal starting from readily available compounds.Herein, we described a catalyst-free α-C–H amination of cyclic amines with *N*-chloro-*N*-sodio-carbamate under the visible light irradiation. The *N*-iodo succinimide (NIS) additive can generate the iminium intermediate in situ, which would then initiate the polar-radical relay cycle in a highly controlled manner. A broad range of α-amino cyclic amines were readily accessed with excellent regioselectivity. This protocol applied the functionalization of biologically relevant complexes.

Poster Presentation : **ORGN.P-406**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of *β*-^{15}N-labeled aliphatic azides using TfNN^{15}N

Sungduk Kwak, Ji Hye Lee, Hyeok-Jun Kwon*, Hogyu Han*

Department of Chemistry, Korea University, Korea

Azides are infrared (IR) probes that are important for structure and dynamics studies of proteins. However, they often display complex IR spectra because of Fermi resonances and multiple conformers. To weaken the Fermi resonance and thereby allow more accurate IR spectral analysis, isotopic substitution of azides can be used. We synthesized TfNN^{15}N, a *γ*-^{15}N-labeled diazo-transfer reagent that was used to prepare AlaN^{15}NN, a *β*-^{15}N-labeled aliphatic azide. It was found that a frequency red-shift of *β*-^{15}N-labeled azide is large enough to overcome spectral interference by Fermi resonance, which is useful to reveal the absence and presence of its weak signal for AlaN^{15}NN and AlaNNN, respectively, in 2DIR spectra.

Poster Presentation : **ORGN.P-407**

Organic Chemistry

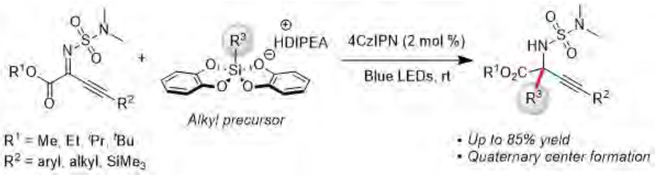
Event Hall FRI 11:00~13:00

Synthesis of α-quaternary amino acid derivatives via photoredox-catalyzed alkyl radical addition to β,γ-alkynyl-α-imino esters

Juyeong Kim, Ansoo Lee*

Brain Science Institute, Korea Institute of Science and Technology, Korea

Unnatural α-amino acids are a crucial class of building blocks in the synthesis of modified peptides to improve their bioactivity and metabolic stability. In particular, quaternary α-amino acids, also called α,α-disubstituted amino acids, are valuable structures widely used to obtain enhanced and unusual biological properties due to conformational constraint, which restricts the structures of their peptides and proteins.[1] Given the biological importance of quaternary α-amino acids, various strategies have been developed for their construction, including the Petasis and O'Donnell reaction. Since the advance of modern photoredox chemistry, visible-light driven generation of C-centered radicals under mild conditions has emerged as a powerful strategy for the selective C-C bond constructions..[2] In particular, single electron transfer (SET) events of photoredox catalysts with radical precursors such as carboxylic acids, organoborates, organosilicates, and 4-alkyl-1,4-dihydropyridines (alkyl-DHPs) allows to generate readily C(sp3)-centered radicals. Herein we report that alkyl bis(catcholato)silicates as C(sp3)-centered radical precursors are highly efficient to produce α-quaternary amino acid derivatives via selective 1,2-addition to β,γ-alkynyl-α-imino esters, which could potentially undergo both 1,2- and 1,4-additions.[1] Boibessot, T.; Benimelis, D.; Meffre, P.; Benfodda, Z. Amino Acids. 2016, 48, 2081-2101.; Wang, Y.; Song, X.; Wang, J.; Moriwaki, H.; Soloshonok, V. A.; Liu, H. Amino Acids. 2017, 49, 1487-1520.[2] Prier, C. K.; Rankic, D. A.; MacMillan, D. W. C. Chem. Rev. 2013, 113, 5322−5363.; Skubi, K. L.; Blum, T. R.; Yoon, T. P. Chem, Rev, 2016, 116, 10035-10074.



R^1 = Me, Et, ^{i}Pr, ^{t}Bu
R^2 = aryl, alkyl, $SiMe_3$

- *Up to 85% yield*
- *Quaternary center formation*

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Poster Presentation : **ORGN.P-408**

Organic Chemistry

Event Hall FRI 11:00~13:00

The effects of PEG hydrogel crosslinking density on drug diffusion

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Jeju National University, Korea
[1]*Department of Chemistry and Cosmetics, Jeju National University, Korea*
[2]*Department of Chemistry, Jeju National University, Korea*

Hydrogels, which have excellent biocompatibility and fluidity, can be used as medical products such as capsules or dressings. Among these hydrogels, synthetic PEG hydrogels can be modularized by design, unlike natural hydrogels, to control functions or structural properties. However, information related to the change by various factors of the hydrogel is not sufficient. In this study, changes in the diffusion of drug according to molecular weight of the substance and PEG backbone, concentration of buffer solution, and pH conditions were investigated. Various equivalents of multi-Arm, PEGs and fluorescent drug were prepared and photopolymerized under UV light. Then, it was swollen in a buffer solution of various pH. Finally, the diffusion of hydrogels was measured with an fluorescence spectrophotometer, and compared with the stiffness and viscoelasticity of the hydrogel which were measured with a rheometer.

Poster Presentation : **ORGN.P-409**
Organic Chemistry
Event Hall FRI 11:00~13:00

Control of Dopamine Surface Chemistry by *N*-Methylation

Yejin Kim, Min Kim, Sung Min Kang*

Department of Chemistry, Chungbuk National University, Korea

Dopamine has been of interest as a surface coating agent, because of its material-independent surface coating capability. Since the first report of dopamine surface chemistry, various dopamine derivatives have been synthesized to elucidate the origin of the surface coating property. Herein, the effect of *N*-methylation on dopamine surface chemistry is reported. Dopamine *N*-methylation improves the coating rate by increasing the nitrogen nucleophilicity, whereas the *N*,*N*-dimethylation reduces the surface coating property.

Poster Presentation : **ORGN.P-410**

Organic Chemistry

Event Hall FRI 11:00~13:00

Remodelling of (Aza)Indole skeleton to substituted pyridines via Aldol condensation/ring opening reaction

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Division of Chemistry, Seoul National University, Korea

There are many methods have been known in the literature for the synthesis of substituted pyridine, with various functional groups, includes esters, acid, phosphonates and sulfonates. In general, the pyridine ester are easily synthesized from Bohlmann-Rahtz pyridine synthesis. Following Bohlmann-Rahtz pyridine synthesis, great number of methodology development to build a substituted pyridine 3-carboxylic acid appeared in the literature. On the other hand, sulfonates and phosphonates embodied pyridines are prepared from coupling reactions using metal catalysis. This strategy represents the use of halo arenes reaction with their corresponding aryl sulfonyl chloride or diethylphosphonate. Recently our group have been reported a biomimetic approach for the synthesis of substituted meta-aminoaryl nicotinates or pyridine 3-carboxylate from 3-formyl (aza)indoles. Unlike previous studies, our methodology demonstrated the in situ generation of enamine from ethyl propiolates thus reaction with 3-formyl (aza)indoles to render ortho unsubstituted pyridines. As part of our ongoing exploration and the use of various enamines synthesized from β-keto electron withdrawing groups such as ester, phosphonates and sulfonates reaction with 3-formyl (aza)indoles to furnish highly substituted pyridines with various electron withdrawing group on the 3-position of the pyridine ring. In this context we will be designated a single methodology reaction for accessing aryl amine conjugated substituted pyridines (embodied with esters, sulfonates and phosphonates) in virtue of remodeling of 3-formyl (aza)indole through aldol condensation and ring opening reaction.

Poster Presentation : **ORGN.P-411**

Organic Chemistry

Event Hall FRI 11:00~13:00

Blue thermally activated delayed fluorescence emitter using multiple electron donors and a rigid electron acceptor

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Department of Chemistry, Seoul National University, Korea
[1]*Department of Chemistry & Cosmetics, Jeju National University, Korea*
[2]*Department of Chemistry, Jeju National University, Korea*

Thermally activated delayed fluorescence (TADF) is a promising concept to improve internal quantum efficiency (IQE) and external quantum efficiency (EQE) of organic light-emitting diodes (OLEDs). A rigid molecular structure is required to enhance the IQE and sharpen the emission spectrum. Recently a rigid 5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene (OBO) as an electron acceptor was utilized for synthesizing TADF emitters which exhibited high EQEs and narrow full width at half maximum (FWHM). We used multiple 3,6-di-*tert*-butyl-9H-carbazoles as electron donors and the OBO as the electron acceptor to develop 9,9',9''-(5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene-3,7,11-triyl)tris(3,6-di-*tert*-butyl-9H-carbazole) (OBOttBuCz). The OBOttBuCz showed a maximum emission wavelength (λ_{max}) of 426 nm, FWHM of 41 nm, and the energy difference between singlet and triplet states (ΔE_{ST}) of 0.16 eV which is sufficient value to emit TADF emission. Also, 10% doped film in bis[2-(diphenylphosphino)phenyl] ether oxide (DPEPO) exhibited a high PLQY of 90% and distinct TADF emission. Therefore, an OLED device using the OBOttBuCz showed a high EQE of 23% and blue color emission of 460 nm.

Poster Presentation : **ORGN.P-412**

Organic Chemistry

Event Hall FRI 11:00~13:00

Mild and Ligand-Free NiH-catalyzed Hydroacylation of Vinylarenes with Acyl Fluorides

Jihye Kim, Jieun Jang[1], Kwangmin Shin[*]

Department of Chemistry, Sungkyunkwan University, Korea
[1]*chemistry, Sungkyunkwan University, Korea*

α-Arylated ketones are frequently found in many natural products pharmaceuticals, and bioactive molecules. As a result, significant effort has been devoted to develop efficient synthetic protocols for the construction of these structural motifs. Among these strategies, metal-hydride catalyzed hydroacylation of vinylarenes with acyl electrophiles has been extensively studied in recent years. Despite these advances, however, the acyl source for hydroacylation is still highly restricted to acid anhydrides. [1-3] Thus, it remains highly desirable to develop a complementary method that enables the use of other type of acyl electrophiles. Acyl fluorides are well known to have a fine balance between stability and reactivity.[4]The use of these attractive acyl electrophiles in metal hydride-catalyzed hydroacylation, however, has been underdeveloped. [5] Herein, we report a nickel hydride-catalyzed hydroacylation of vinylarenes with acyl fluorides under ligand-free conditions.[6] Along with ligandless conditions, the present catalytic protocol is distinguished by its mild conditions, simple catalytic setup, and broad substrate scope. Furthermore, the reaction can be performed on a gram scale without the use of a glovebox, demonstrating the practicality of the present hydroacylation method.

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5. Ueda, Y.; Iwai, T.; Sawamura, M. Chem. Eur. J. 2019, 25, 9410-9414.
6. Kim, J.†; Jang, J.†; Shin, K. Manuscript in preparation. († equally contributed)


O
F
+
Ar
Ni-H
O
Ar
acyl fluoride
vinylarene
no added ligand
mild reaction conditions
wide substrate scope
α-arylated ketone

Poster Presentation : **ORGN.P-413**

Organic Chemistry

Event Hall FRI 11:00~13:00

Access to β-Lactams via Iron-Catalyzed Olefin Oxyamidation Enabled by the π-Accepting Phthalocyanine Ligand

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[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*
[2]*Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea*

Herein, we report the development of an iron-catalyzed olefin oxyamidation by utilizing tethered dioxazolones as the nitrenoid precursor to produce valuable β-lactam scaffolds. Mechanistic studies revealed that a relatively strong π-accepting ability of the phthalocyanine ligand is critical in generating the key triplet iron-imidyl radical intermediate to enable the 4-exo-trig-lactamization with the incorporation of oxygen nucleophiles at high diastereoselectivity. This cyclization approach was readily extended to the highly efficient γ-lactam synthesis (TON > 300).

Poster Presentation : **ORGN.P-414**

Organic Chemistry

Event Hall FRI 11:00~13:00

Chain Walking as a Strategy for Iridium-Catalyzed Migratory Amidation of Alkenyl Alcohols to Access α-Amino Ketones

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While an accessing valuable nitrogen-containing compounds is an appealing field in organic chemistry, catalytic carbon—nitrogen bond formation of hydrocarbons is a fascinating synthetic tool. Although a number of approaches to generate an α-amino carbonyl scaffold have been developed well, however, functionalization at remote and unfunctionalized aliphatic sites installing an amino group remains underdeveloped. Herein, we introduce the tandem iridium catalyzed redox-relay amidation of alkenyl alcohols via chain walking and metal-nitrenoid transfer, which eventually offers a new synthetic route to various α-amino ketones with excellent regioselectivity. Experimental result that unrefined isomeric mixture of alkenyl alcohols can be utilized as available starting materials in this system giving the additional virtue in synthetic utility, giving the regioconvergent amidated ketones. Detailed tandem process involving two key components of redox-relay chain walking and intermolecular nitrenoid transfer assisted by hydrogen bonding was proposed via mechanistic experiment and density-functional theory (DFT) calculation, thus representing the competence of Ir catalysis for the olefin migratory C—N coupling with high efficiency and exquisite selectivity.

Poster Presentation : **ORGN.P-415**

Organic Chemistry

Event Hall FRI 11:00~13:00

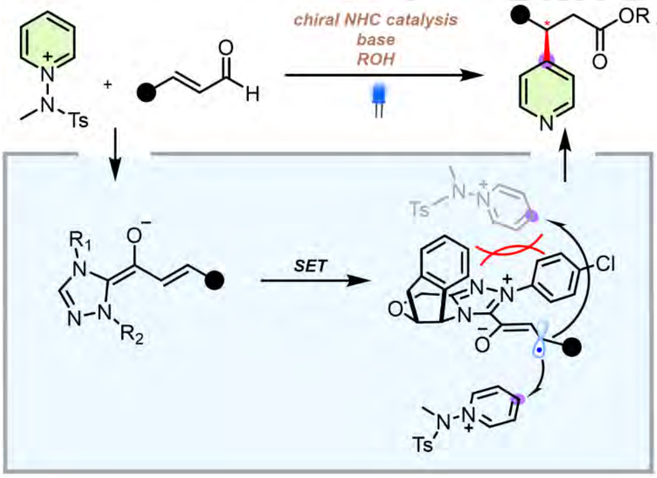
Enantio- and C4-selective Functionalization of Pyridinium Salts through N-Heterocyclic Carbene Catalysis

Seonghyeok Hong, Sungwoo Hong[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

A catalytic method for the functionalization of pyridine derivatives with enantioselectivity and C4-selectivity has not been developed yet. Herein, we report an efficient method for the asymmetric functionalization of pyridinium salts with enals that involve N-heterocyclic carbene (NHC) catalysis with excellent control over enantioselectivity and pyridyl C4-selectivity. The key strategy of control enantioselectivity entails enhancing interactions between pyridinium salt and the chiral NHC-bound homoenolate with hexafluorobenzene which effectively differentiates the two faces of the homoenolate radical. Without external thermal conditions, room temperature is sufficient for this conversion, and reaction efficiency is further accelerated by photo-irradiation. This methodology demonstrates broad functional group tolerance and permits facile access to a varied range of enantioenriched β-pyridyl carbonyl compounds under metal- and photocatalyst-free conditions.



Poster Presentation : **ORGN.P-416**

Organic Chemistry

Event Hall FRI 11:00~13:00

Multivalent Interaction using disulfide formation-induced Self-Assembly inside Mitochondria for Senolytic Effect

Sangpil Kim, Ja-Hyoung Ryu[1,*], Dohyun Kim[1]

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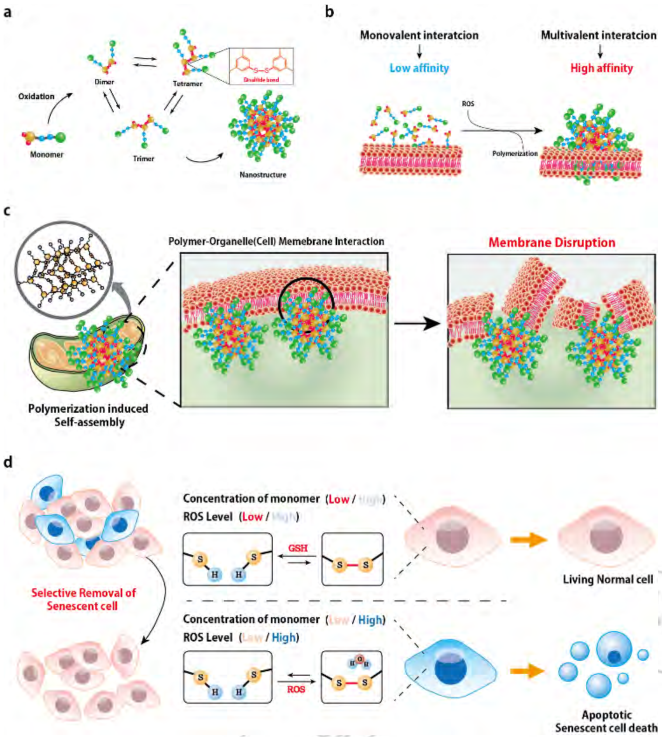
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

The intracellular biomacromolecules including proteins, DNA, and polysaccharides, play an important role to perform cellular function. Theses macromolecules are synthesized by multicomponent self-assembly of building blocks such as amino acids, nucleotides, and monossacharides. Such an assembly relies on interaction of individual building blocks to create complex and high ordered structure. By mimicking the natural system, we found that formation of disulfide bond give a great platform to form multicomponent assembled structure for multivalent interaction with bio-macromolecules. Thus, we developed multicomponent self-assembly using disulfide bond to interact with mitochondrial membrane via multivalent interaction for inducing dysfunction of mitochondria, leading to apoptosis of senescent cells specifically. This polymerization shows great potential for senolytic treatment with selective removal of senescent cells.


a
Oxidation
Monomer
Dimer
Trimer
Tetramer
Disulfide bond
Nanostructure
b
Monovalent interatcion
Low affinity
Multivalent interatcion
High affinity
ROS
Polymerization
c
Polymer-Organelle(Cell) Memebrane Interaction
Membrane Disruption
Polymerization induced Self-assembly
d
Selective Removal of Senescent cell
Concentration of monomer (Low / High)
ROS Level (Low / High)
GSH
S
H
S
H
S
S
Living Normal cell
Concentration of monomer (Low / High)
ROS Level (Low / High)
ROS
Apoptotic Senescent cell death

Poster Presentation : **ORGN.P-417**

Organic Chemistry

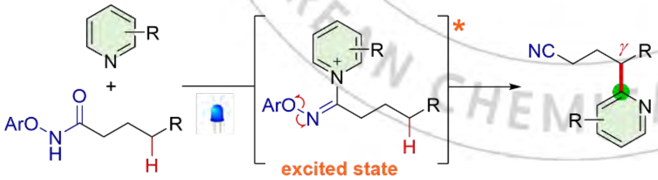
Event Hall FRI 11:00~13:00

Remote C-H Pyridylation via Direct Photoexcitation of In Situ Generated O-Aryl Oxime Pyridinium Salts

Changha Kim, Sungwoo Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

A direct site-selective C-H functionalization of pyridine is a useful reaction for the modification of pyridine-based complex. Herein, we report C2 selective pyridylation of hydroxamate via in situ generation of a direct photoexcitable O-aryl oxime pyridinium salts. Oxime pyridinium salts can be photoexcited by irradiation of visible light without the use of external photocatalyst, which could then induce photolytic N-O cleavage to form iminyl raidcals. The iminyl radicals can generate carbon-centered radical which undergoes intramolecular addition to C2 position via 1,5-HAT. This direct-photoexcited radical addition mechanism was further demonstrated by mechanistic experiments and DFT calculation. This method tolerates broad functional group under mild and catalyst-free conditions.



- *PC-free direct photoexcitation*
- *γ-C-H selective remote coupling*
- *in situ activation of pyridines*
- *ortho-selective addition*

Poster Presentation : **ORGN.P-418**

Organic Chemistry

Event Hall FRI 11:00~13:00

Development of First-in-class Drugs for Triple Negative Breast Cancer based on Antibody-mimic Recombination Proteins

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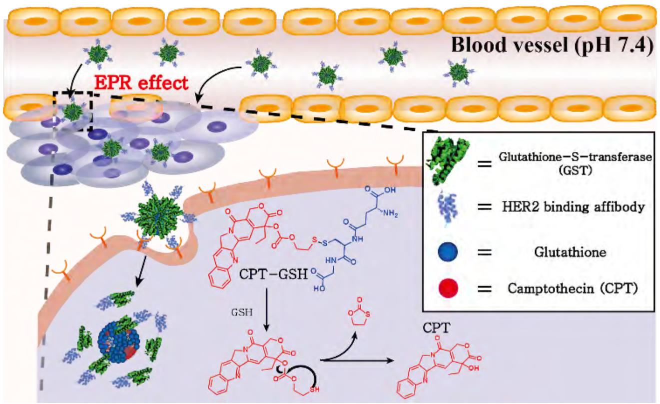
TNBC, the term triple-negative breast cancer, describes a subtype of breast cancer that lacks expression of estrogen (ER), progesterone receptor (PR), and human epidermal growth factor 2 receptor (HER2). In recent, Antibody-drug conjugate (ADC) is emerging as a promising agent for treating TNBC. It enables selective delivery to tumors by using the properties of antibodies that recognize specific antigens. However, developing ADCs requires overcoming high hurdles in synthesis and purification with antibodies. Therefore, herein, a novel TNBC treatment system has been developed that overcomes the disadvantages of ADC. The synthesis and purification process was shortened through supramolecular binding using substrate-specific binding. Since this recombinant protein has a binding pocket that can specifically bind to the substrate attached to the linker, the structure of “anticancer drug-linker-affibody attached recombinant protein” can be constructed. The anticancer drug-linker was designed for self-assembly. The hydrophobic drug is located on the core, and the hydrophilic substrate is exposed to the surface of a self-assembly form, and when recombinant protein is bound to this surface, a "protein-coated self-assembled structure" can be formed which can target TNBC. The camptothecin (CPT) was modified to form a disulfide bond with cysteine of Glutathione (GSH). It can convert to the original parent CPT drug when the disulfide bond is cleavaged. GSH was used as the substrate, and Glutathione-S-Transferase (GST) having a binding pocket with GSH was used as the recombinant protein. The GST used in this study has an EGFR binding affibody that can bind to the EGFR receptor overexpressed in TNBC, and thus has a targeted ability against TNBC.


Blood vessel (pH 7.4)
EPR effect
= Glutathione−S−transferase (GST)
= HER2 binding affibody
= Glutathione
= Camptothecin (CPT)
CPT−GSH
GSH
CPT

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Poster Presentation : **ORGN.P-419**

Organic Chemistry

Event Hall FRI 11:00~13:00

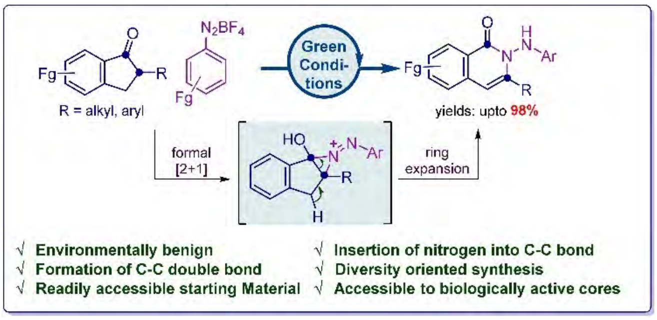
Green and Efficient Constructive Skeletal Editing: Synthesis of 2-(Phenylamino)isoquinolin-1(2*H*)-one and Applications

Mohammed Anif pasha, Seunghoon Shin[1,*]

CHEMISTRY, Hanyang University, Korea

[1]*Department of Chemistry, Hanyang University, Korea*

Over the decades, diazonium salts were used as arylation agents due to their easy accessibility. Recently, the “molecular editing” concept is being formulated as has a method of changing the structure of late-stage intermediates. In this context, skeletal editing of an aromatic system by nitrogen insertion is relatively under-explored. Building on this backdrop, an efficient and green protocol for direct constructive skeletal editing by inserting diazonium salt into benzo-fused cyclic ketones has been developed for the high yielding synthesis of biologically and pharmaceutically important isoquinolin-1(2*H*)-one derivative. Herein, a wide range of α-substituted 1-indanones treated with a variety of aryl diazonium salts at 50 ^{o}C in acetonitrile for the 2-8 h furnishes 2-(phenylamino)isoquinolin-1(2*H*)-one up to 98% yield.**Acknowledgment**This work was financially supported by National Research Foundation (NRF-2012M3A7B4049653, NRF-2014-011165 and NRF-2017R1A2B4010888), Center for New Directions in Organic Synthesis (CNOS) and Sansung Science and Technology Foundation (SSTF-BA1602-10).**References:**1. Anif Pasha, M.d.; Shin, S. *manuscript under submission*.2. Levin, M.D et al. a) *Nature*, **2021**, *593*, 223. b) *J. Am. Chem. Soc*. **2021**, *143*, 11337.3. Antonchick, A.P et al. *J. Am. Chem. Soc*. **2021**, *143*, 18864.4. Sarpong, R. et al. *Nature*, **2018**, *564*, 244.



Poster Presentation : **ORGN.P-420**
Organic Chemistry
Event Hall FRI 11:00~13:00

Photoluminescent and Electrochemiluminescent Detection of Hg^{2+} Ion with a Boronic acid Functionalized Iridium(III) Complex

Kyoung-Rok Kim, Jong-in Hong*

Division of Chemistry, Seoul National University, Korea

Electrogenerated chemiluminescence (ECL) is a luminescent process through sequential electron transfers to and from chemicals on an electrode surface. The ECL assay is advantageous compared to conventional fluorescence assay due to its high sensitivity, low background signal, and good reproducibility. Furthermore, it does not require a complicated procedure, condition and large equipment for analysis. For these reasons, ECL assay is considered as a powerful technique for on-site real sample monitoring systems.Mercury(II) ion (Hg^{2+}) is well-known as an persistent, bio-accumulative, and toxic (PBT) substance, which is threatening human health and the ecosystem. It is easily absorbed into the body through the cell walls of the skin, respiratory tract, and biological gastrointestinal tract due to the difficulty to sense it through human sensory organs by its colorless, tasteless, and odorless nature. When Hg^{2+} is assimilated into the human body, it causes damages of the central nervous system and endocrine glands. Furthermore, chronic exposure to Hg^{2+} induces various diseases such as Minamata, acrodynia, Alzheimer's disease and Hunter–Russell syndrome. For these reasons, the U. S. Environmental Protection Agency (EPA) recommended the maximum level of mercury in drinking water to be 10 nM. Herein, we report a new photoluminescent and electrochemiluminescent chemodosimeter based on a cyclometalated Ir(III) complex for the determination of Hg^{2+} ion. The probe 1 was rationally designed for the selective detection of Hg^{2+} ion using the transmetalation reaction of phenylboronic acid with Hg^{2+} ion. It showed prompt response, high sensitivity, and remarkable specificity toward Hg^{2+}. Details of photophysical and electrochemical properties will be presented.

Poster Presentation : **ORGN.P-421**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of NHC-Iridium Catalysts for various hydrogen-mediated reactions

<u>Heemin Byeon</u>, Mi-hyun Lee, Hye-Young Jang[1,*]

Department of Energy System Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

N-Heterocyclic carbene (NHC) ligands, strong σ donor form stable transition metal complexes. In addition to giving stability to the complex, NHCs involving various functional groups can be easily synthesized and incorporated into the complex. In this study, we synthesized bimetallic NHC-Ir(III) catalysts using aromatic ring bridged ligands. Since Iridium catalysts are known to be effective in hydrogen-mediated reactions, these were applied to transfer hydrogenation, dehydrogenation, and reactions involving borrowing hydrogenation approaches.

Poster Presentation : **ORGN.P-422**

Organic Chemistry

Event Hall FRI 11:00~13:00

Transition-Metal-Catalyst-Free Synthesis of ß-Ketonitriles using Acetonitrile and Amides

Jonghoon Oh*, Sunwoo Lee*, Myeong Seong Park[1], Suhyeon Park

Department of Chemistry, Chonnam National University, Korea
[1]*Department Of Chemistry, Chonnam National University, Korea*

Beta-ketonitriles is one of the most valuable functionality in organic synthesis because it can readily be converted a variety of heterocyclic compounds. Various synthetic methods for beta-ketonitrile have been developed. Among them, transiton-metal catalyzed carbonylative coupling, electrophilic cyanation, and acyl substitution reaction are straightforward and most often employed tools for the preparation of beta-ketonitrile. However, there is no report of the acyl substitution reaction of amides. Herein we report the synthesis of beta-ketonitrile from the reaction of amides and acetonitrile. We found that N-phenyl-N-tosyl benzamides reacted with acetonitrile in the presence of LiHMDS, the corresponding benzoylacetonitriles were formed in good yields.

Poster Presentation : **ORGN.P-423**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Multi-targeting Drug Delivery System Containing Two Anticancer Agents

Hui Li, Injae Shin[1,*]

Chemistry, Yonsei Univerisity, Korea

[1]*Department of Chemistry, Yonsei University, Korea*

Over the past several decades, numerous potential chemotherapeutic agents have been developed to treat tumors. A major goal of these efforts is the discovery of safe and efficacious anticancer drugs, which have enhanced selectivity against cancer cells over normal cells and, thus, display minimal side effects. To improve tumor selectivity, we designed and synthesized a triple-targeting delivery system (Oct-FK(PBA-Az)-Dox) carrying two anticancer agents (apoptozole (Az) and doxorubicin (Dox)). The results showed that both of the anticancer agents in this substance are released in the presence of hydrogen peroxide and cathepsin B, both of which are produced at high levels in cancer cells.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-424**
Organic Chemistry
Event Hall FRI 11:00~13:00

A Novel OFF-ON Fluorescent probe for detecting Methylglyoxal

Yuvin Noh, Jinwoo Shin, Subin Son, Ji Hyeon Kim, Jusung An, Ilwha Kim, Youmi Choe, Soyu Zi, Jaewon Kim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Methylglyoxal (MGO) is a reactive cytotoxic dicarbonyl compound mainly formed as a byproduct of glycolysis, and its pathological importance is increasing due to its pivotal role as a precursor of advanced glycation end products (AGEs), which is overexpressed as in various diseases, including aging disorders, diabetic complications, and chronic inflammation. In the current work, a novel MGO-sensitive coumarin-based fluorophore (CM1) was rationally designed through tailoring the o-phenylenediamine (OPD) moiety, an MGO-sensitive trigger, to achieve intramolecular photo-induced electron transfer (PeT) for “OFF-ON” type fluorophore. OPD moiety of CM1 is transformed to 2-methylquinoxaline in reaction to MGO and loses its ability as a PeT ligand to regain high fluorescence for the "OFF-ON" fluorophore. Based on solution-based results, an unprecedented selectivity toward MGO than competitive analytes was accomplished without any noticeable off-target sensing. The current findings suggest the potential of using an MGO-sensitive probe with exceptional selectivity as a promising diagnostic approach for MGO related disease.

Poster Presentation : **ORGN.P-425**

Organic Chemistry

Event Hall FRI 11:00~13:00

Bromoacetate Olefination Protocol for Norbixin and Julia−Kocienski Olefination for Its Ester Syntheses

Aleksei Golikov, Sangho Koo*

Department of Chemistry, Myongji University, Korea

Norbixin 1 was expeditiously synthesized by coupling of ethyl bromoacetate with C20 dialdehyde 6 and subsequent double elimination of the protected hydroxyl groups and bromine atoms of the coupling bromohydrin product. Synthesis of norbixin ethyl ester 2 by Julia−Kocienski olefination of novel C7 benzothiazolyl-sulfone 11 and C10 2,7-dimethyl-2,4,6-octatrienedial 12 also was shown. These two concise pathways led to 35% and 36% overall yield of norbixin 1 and norbixin ethyl ester 2, respectively.

Poster Presentation : **ORGN.P-426**

Organic Chemistry

Event Hall FRI 11:00~13:00

An effective one-pot reaction that converts carbohydrates into pyrrole-2-cavaldehyde

Hyein Kim, Sangho Koo[1,*]

Myongji University, Korea

[1]*Department of Chemistry, Myongji University, Korea*

A method for synthesizing a pyrrole structure from glucose without going through fructose in one-pot was studied. By heating glucose and the primary amine at 90oC using a DMSO solvent under oxalic acid conditions, a pyrrole-structured Pyrraline compound can be synthesized through an additional cyclization reaction through an amine group accompanied by N-glycosylation and Amadori reaction and Dehydration.

Poster Presentation : **ORGN.P-427**

Organic Chemistry

Event Hall FRI 11:00~13:00

Total synthesis of grifolin via C-alkylation of 5-methylcyclohexane-1,3-dione

Huisu Yeo, Han Seunghyo, Sangho Koo[1,*]

Organic chemistry, Myongji university, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Grifolin is a biological active natural product that can be extracted from mushroom, Albaterus dispansus. It prevents early-stage tumor deformation by suppressing or blocking the cancer cell promoting process.The total synthesis of grifolin, which has a resorcinol core with farnesyl chain, has been studied by research groups. When synthesizing grifolin using Fridel-craft alkylation, there are problems of regio-chemistry and cyclization. Our synthesis proposal is to use 5-methylcyclohexane-1,3-dione instead of resorsinol. We studied O-alkylation vs C-alkylation of dione and farnesyl chain, and the resulting C-alkylation product underwent aromatization. Our method can show and efficient way to synthesize grifolin, the details are described in the poster.

Poster Presentation : **ORGN.P-428**
Organic Chemistry
Event Hall FRI 11:00~13:00

The Effect of Ring-ortho Substituents on the Configuration of Carotenoid Polyene Chains as Molecular Wires

Chanyoung Boo, Sangho Koo[1,*]

Department of Chemistry, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Carotenoids containing phenyl substituents to the polyene chain provide not only improved stability, but also diverse electron-conducting abilities to the chain. We studied the effect of ring-ortho substituents on configuration of carotenoids as a molecular wires. The 2,6-dimethyl substituents in the terminal rings secure an all-(E)-polyene chain. Contrastively, the 9-(Z)-configuration was exclusively obtained in the carotenoid polyene chain irrespective of olefination and disconnection methods for terminal ortho-unsubstituted benzene rings. We measured the conductance of the above carotenoids. The single molecular conductance of the pure 9-(Z)-carotene was measured for the first time to be 1.53 × 10−4 ± 6.37 × 10−5G0, whose value was 47% that of the all-(E)-carotene ((3.23 × 10−4) ± (1.23 × 10−4) G0).

Poster Presentation : **ORGN.P-429**

Organic Chemistry

Event Hall FRI 11:00~13:00

Furan oxidation by Mn(III)/Co(II) catalysis-application to benzofuran synthesis

Hongyu Zhu, Sangho Koo[1,*]

Organic chemistry, Myungji University, China
[1]*Department of Chemistry, Myongji University, Korea*

In order to explore the oxidation reaction catalyzed by manganese acetate, a new furan rearrangement reaction was discovered. The heterocyclic small molecule compounds with medical activity were obtained through this reaction. For this novel furan rearrangement reaction, we explored the mechanism of the reaction by changing the reaction conditions and the structure of the substrates. It was found that the rearrangement reaction is related to the formation of peroxy radical intermediates.The novel furan rearrangement reaction discovered and explored has the advantages of easy preparation, simple operation, rich functional groups and with many applicabilities, which provides a new method and a new idea for the synthesis of natural active compounds.

Poster Presentation : **ORGN.P-430**

Organic Chemistry

Event Hall FRI 11:00~13:00

Furan oxidation by Mn(III)/Co(II) catalysts – application to benzofuran synthesis

Yifan Zheng, Sangho Koo[1,*]

Department of Chemistry, Myungji University, China

[1]*Department of Chemistry, Myongji University, Korea*

Furans containing a β-ketoester group at 2-position undergo oxidative ring-opening by Mn(III)/Co(II) catalysts under an O2 atmosphere to produce 1,4-dicarbonyl moieties through an endoperoxide intermediate, which consecutively cyclized with the β-ketoester unit to afford 4-hydroxy-2-cyclohexen- 1-ones. This oxidation/cyclization products were efficiently transformed into versatile benzofuran derivatives after consecutive aromatization and Paal–Knorr reaction.

Poster Presentation : **ORGN.P-431**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fast Assembly and High-Throughput Screening of Structure and Antioxidant Relationship of Carotenoids

Gaosheng Shi, Sangho Koo[1,*]

Department of Energy Science and Technology, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

C20 heptaenyl diphosphonate 4 was prepared for one-pot synthesis of carotenoids 1. Olefination with various aromatic aldehydes allowed fast assembly of the corresponding carotenoids. The SAR of carotenoids was investigated by high throughput screening of ABTS and DPPH assays and their hierarchical clustering analysis. Antioxidant activity of carotenoids increased with the number of electron-donating substituents. Carotene 1a with multiple electron-donating substituents was most proficient, which showed better radical scavenging activities than β-carotene and lycopene.

Poster Presentation : **ORGN.P-432**

Organic Chemistry

Event Hall FRI 11:00~13:00

Heavy Atom Free BODIPY Based Photosensitizers Exhibiting Enhanced Triplet State Generation by Radical Pair Intersystem crossing

You Rim Lee, Sungnam Park[1,*], Juyoung Yoon[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

[1]*Department of Chemistry, Korea University, Korea*

Image-guided photodynamic therapy (PDT) is a hot research area in the field of cancer theranostics. Previously studied Boron-dipyrromethene (BODIPY) derivatives incorporated with heavy-atoms are well known for their large molecular absorption coefficients and enhanced intersystem crossing (ISC) process, but heavy atoms possess problems such as short triplet excited state lifetime and dark toxicity which limits the application in image-guided PDT. In the attempt to overcome these drawbacks, heavy atom free photosensitizers, BDP-8 and BDP-9, based on acceptor-donor-acceptor (A-D-A) structure with BODIPY acceptor and phenoxazine donor were synthesized and studied. These photosensitizers displayed large molecular absorption coefficients with aggregation-induced emission (AIE) in the red region which is beneficial for bioimaging. They also showed excellent triplet excited state generation through the radical-pair ISC (RP-ISC) pathway leading to enhanced reactive oxygen species (ROS) production. Furthermore, the nanoparticles of the photosensitizers demonstrated excellent biocompatibility and ROS generation upon light irradiation. In particular, in vitro and in vivo study of BDP-8 nanoparticles exhibited notable tumor targeting ability and ROS generation, providing an insight in molecular design of potential image-guided PDT agents.

Poster Presentation : **ORGN.P-433**

Organic Chemistry

Event Hall FRI 11:00~13:00

Demonstration of Curved β-Thiopeptide

Jungwoo Hong, Jaewook Kim, Hee-Seung Lee*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The oligopeptide of trans-ACPC(2-aminocyclopentanecarboxylic acid), one of the most well-known β-amino acids, is prone to induce helical structure. Its 12-membered intramolecular hydrogen bonding pattern is nearly absolute, with no exceptions within our knowledge up to date. The stable helical propensity of ACPC oligopeptide makes ACPC a very useful building block for helical peptides, but it also reduces structural and conformational diversity. To establish thioamide as a designable and controllable platform as peptidomimetics, herein we report a series of thioamide analogs of ACPC oligopeptide. Unlike monotonous pattern of ACPC oligopeptide, those thiopeptide series have unique intra- and intermolecular hydrogen bonding pattern. Also, in some cases, we succeeded to realize the helical peptide with 3-dimensional curvature. Base on those results, we have demonstrated the possibility of thioamide as the tool of structural regulation of helical peptides.

Poster Presentation : **ORGN.P-434**

Organic Chemistry

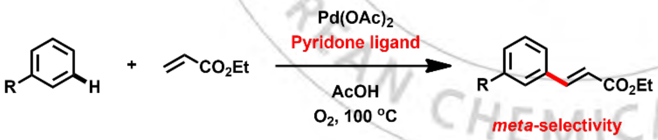
Event Hall FRI 11:00~13:00

Ligand-enabled meta-selective C–H Alkenylation of Functionalized Arenes

Jung Min Joo*, Jisu Kim

Department of Chemistry, Pusan National University, Korea

The development of regioselective transition-metal-catalyzed reactions can be achieved by developing new ligands. We synthesized a new ligand which has a pyridone moiety in the ligand framework. With this ligand, we were able to activate the meta-position of arenes, which was not readily activated because of the electron-deficient nature, and demonstrate *meta*-selective C–H alkenylation. Several mechanistic studies were performed, including kinetic order, deuterium labelling, and DFT computational analysis to investigate the properties of pyridone ligands. Through these studies, it was found that the pyridone ligand acted as an internal base, reducing the activation energy of the C-H cleavage at the electron-deficient site. The substrate scope including a variety of substituted arenes and polycyclic arenes will be described.



Poster Presentation : **ORGN.P-435**

Organic Chemistry

Event Hall FRI 11:00~13:00

Development of dual-channel fluorescent probe for tracking H_2S and NTR in hypoxic cancer cells

Shin A Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Hydrogen sulfide (H_2S) is a crucial redox molecule and endogenous gas transmitter, physiological and cellular protective functions in biological systems. Nitroreductases (NTR) are flavoenzymes that catalyze the NAD(P)H-dependent reduction of the nitro group on nitroaromatic compounds and play a key role in the detoxification of carcinogens. Recently, some literatures have reported that the NTR activity and H_2S increase under hypoxia in cancer cells.In our research, we developed the dual-channel fluorescent probe **1** for imaging H_2S and NTR in hypoxic conditions. The probe **1** was constituted in a combination of fluorophore, nitrobenzoxadiazole (NBD) and nitrobenzyl moiety. Probe **1** showed emission at 475 nm and 547 nm in the presence of H_2S and NTR/NADH, respectively. Moreover, the detection limits of probe **1** for H_2S and NTR were calculated to 1.5 μM and 3.4 ng/mL, respectively. Additionally, encouraged by the excellent photophysical properties, probe **1** was applied to image NTR and H_2S in $CoCl_2$-induced hypoxic HeLa cells with the blue and green channels. This study is ongoing, and we expect probe **1** can be applicable to H_2S and NTR-associated disease models.

Poster Presentation : **ORGN.P-436**

Organic Chemistry

Event Hall FRI 11:00~13:00

NAD(P)H-activable fluorescent probes for the detection of cellular NAD(P)H in various cancer cells

Yujin Cha, Songyi Yoo, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Reduced nicotinamide adenine dinucleotide (NADH) and reduced nicotinamide adenine dinucleotide phosphate (NADPH) are essential coenzymes existed in human cells. NAD(P)H is involved in many biological processes such as energy metabolism, mitochondrial function, biosynthesis, cell death, and aging. In addition, the overexpression of NAD(P)H has been observed in various diseases, including cancer, neoplasia, Parkinson’s and Alzheimer’s diseases. Therefore, NAD(P)H has been considered as a potential target for the diagnosis and the related research fields for drug discovery.In this regard, we developed NAD(P)H-activable fluorescent probes 1 and 2 composed of different intramolecular charge transfer (ICT) acceptor parts possessing different electron withdrawing abilities. In the presence of NAD(P)H, probes 1 and 2 get reduced and exhibit strong ICT emissions at 575 and 640 nm. In biological experiments, probes 1 and 2 showed fluorescence emissions toward cellular NAD(P)H in MDA-MB-231 cells. In addition, the probes displayed fluorescence changes in glucose treated cells where NADH is generated by glycolysis. We expect that the changes will differ depending on cell lines, and our probes could differentiate various cells.

Poster Presentation : **ORGN.P-437**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fluorescent probe targeting lysosomes for simultaneous monitoring of viscosity and nitric oxide

Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Intracellular viscosity is a physicochemical factor that determines the outcome of various biological processes, and nitric oxide (NO) is an essential signalling molecule that controls many cellular processes, including oxidative stress. We previously reported a fluorescent probe that can simultaneously detect intracellular viscosity and NO. As a follow-up study, we intended to investigate the viscosity and nitric oxide of the lysosomes. Herein, we designed and synthesized probe which can target lysosomes and provide simultaneous fluorescence changes to the viscosity and nitric oxide. We presented physiological properties of the probe in a solution and the living cells. The probe showed distinct fluorescence change in response to elevation of viscosity and NO levels. In addition, we are planning to apply the probe to a disease model regarding the changes in NO and viscosity of lysosomes.

Poster Presentation : **ORGN.P-438**

Organic Chemistry

Event Hall FRI 11:00~13:00

Multiple resonance type thermally activated delayed fluorescence (MR-TADF) novel host materials based on silicon derivatives

Dongmin Park, Jongwook Park[1,*], Soo young Park[*]

Department of Materials Science & Engineering, Seoul National University, Korea

[1]*Department of Chemical Engineering, Kyung Hee University, Korea*

Thermally activated delayed fluorescence(TADF) has attracted large attention for next generation organic light-emitting diode(OLED) devices. Theoretically, TADF has an internal quantum efficiency of up to 100% by harvesting triplet energy to singlet energy. Also, Multiple Resonance type TADF(MR-TADF) materials containing boron achieve high external quantum efficiency(EQE) and have a narrow emission spectrum as a result of a rigid frame. However, while many studies about MR-TADF have been conducted on dopant materials, there have been few studies on host materials. Here, we developed 6 host MR-TADF materials based on, 2,12-di-tert-butyl-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene(TDBA). It possesses phenyl and tetrapheny-lsilane, in various positions of TDBA. We designed TDBA-Si, TDBA-Ph as a para-positioned material, and m-TDBA-Ph, m-TDBA-2Ph, m-TDBA-Si, and m-TDBA-2Si as a meta-positioned material. They exhibit high triplet energy of 2.8-2.9 eV in toluene and neat film, making them suitable for energy transfer to a blue dopant. Also, a small energy difference between the singlet and triplet states is enough to occur reverse intersystem crossing. Devices that doped ν-DABNA in each 6 materials could successfully reach good performance by harvesting triplet exciton both host and dopant materials. Also, attaching tetraphenyl-silane makes TDBA core more rigid to get high triplet energy and showes maximum EQE values over 30%. Especially, the emission maximum of dopant was blue shifted 469nm to 465nm by reducing stokes shift of dopant. Thereafter, the Commission Internationale de l’Eclairage (CIE) coordinates changed (0.12,0.11) to (0.13,0.10). Thus, the novel MR-TADF hosts make a good synergetic effect with TADF dopant.

Poster Presentation : **ORGN.P-439**

Organic Chemistry

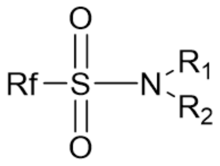
Event Hall FRI 11:00~13:00

Surface tension and interfacial tension of fluorine-containing sulfonamides prepared from perfluoroalkyl sulfonyl halides with alkyl amines

Myoung-Hoon Kim, Eun Sil Kim[1], Surk-Sik Moon*, Byeong Jo Kim[2], Hyun-chul Kang[3], Chan Kyu Kwak[3], Won-Jun Jeong[3]

Department of Chemistry, Kongju National University, Korea
[1]*Kongju National University, Korea*
[2]*R&D Center, Aekyung Chemical, Korea*
[3]*Surfactant material R&D team, R&D Center, Korea*

Sulfonamides were synthesized from perfluoroalkyl sulfonylhalides with alkylamines followed by alkylation with alkyl halides. The structure of each synthesized surfactant was unambiguously characterized by using spectroscopic methods including 1D and 2D NMR (proton, carbon, fluorine, COSY, HSQC, and HMBC) spectroscopy. The surface tension and interfacial tension of each synthesized surfactant were measured and compared with regard to structural variation.



Rf = perfluoroalkyl
R_1 = alkyl
R_2 = alkyl

Poster Presentation : **ORGN.P-440**

Organic Chemistry

Event Hall FRI 11:00~13:00

Rotational Variance of 3D Graph Convolutional Network for Data Augmentation

Jihoo Kim, Yoonho Jeong, Eok Kyun Lee, Won June Kim[1], Insung Choi[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Biology and Chemistry, Changwon National University, Korea*

A new strategy to data augmentation for protein-ligand binding task is proposed based on the rotational-variance characteristic of 3D graph convolutional network (3DGCN). Inactive ligands to human β-secretase 1 are generated by rotating active ligands in the BACE-1 dataset with randomly chosen axes and degrees, and the data-augmented 3DGCN acquires enhanced sensitivity to ligand orientation to human β-secretase 1, suggesting its potential in deep-learning prediction of the optimal binding poses of drug candidates for a given protein target.

Poster Presentation : **ORGN.P-441**

Organic Chemistry

Event Hall FRI 11:00~13:00

Practical Transformation of Aryl hydrazines to *N*-aryl-substituted Azacycles using Titanium Tetrachloride and TBD

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

N-substituted azacycles are one of significant motifs which have been used for widespread application in medicines, dyes and organic materials. Over the years, lots of protocols for preparation of *N*-substituted azacycles have been reported. However, in the previously reported synthetic methods, common starting materials for *N*-substituted azacycles is primary arylamines. The discovery of newly accessible materials to replace primary amines is valuable for in these transformation, and it has inspired to design novel methodology studies. Herein, a new protocol for preparing *N*-substituted azacycles from aryl hydrazines is presented. Initial study suggested that titanium tetrachloride and TBD played an important role in the direct convertion of aryl hydrazine to *N*-substituted azacycles. In this study, reactions in the presence of titanium tetrachloride and TBD successfully afforded a variety of *N*-substituted azacycles including piperidines, pyrrolidines, isoindolines, and tetrahydroisoquinolines in high yields. This method using aryl hydrazines as starting materials can give a novel efficient synthetic approach to synthesize useful *N*-Aryl heterocycle structures.

Poster Presentation : **ORGN.P-442**
Organic Chemistry
Event Hall FRI 11:00~13:00

Facile Direct Synthesis of Amides from Primary Alcohols using Dibromoisocyanuric Acid

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Amide structures are widely found functional groups in nature. For example, peptides contain strong amide bonds to build their structures. And amide structures are crucial parts in a variety of bioactive compounds. Due to their utilities, several synthetic methods such as reaction of carboxylic acids with amines have been developed to prepare amides. Primary alcohols were widely used groups in chemistry, polymer, material science, and pharmacy. Therefore, utilization of primary alcohols is useful challenge for synthetic chemistry. Herein, a novel direct transformation of primary alcohols to amides is described. In the screening study, activated acybromide intermediate was prepared from primary alcohols via treatment of dibromoisocyanuric acid, and then addition of amines and proper bases to the acybromide resulted in successful synthesis of amide structures under mild reaction condition. In this novel procedure, various primary alcohols were directly converted to amides. It can be believed that novel procedure using primary alcohols could give useful strategy for the generation of amide compounds.

Poster Presentation : **ORGN.P-443**

Organic Chemistry

Event Hall FRI 11:00~13:00

Highly Efficient and Stereoselective Mukaiyama Aldol Reaction with Chiral Aziridine-2-carboxaldehyde and Its Synthetic Applications

Nikhil Srivastava, Hyun-Joon Ha[1,*]

Department of Chemistry, Hankuk University of Foreign Studies, India

[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

We successfully synthesized a highly stereoselective β-aziridin-2-yl-β-hydroxy ketones by the Mukaiyama aldol reaction between optically pure 1-(α-methylbenzyl)-aziridine-2-carboxaldehyde and various enol-silanes with $\mathrm{ZnCl2}$ via a chelation-controlled transition state in a highly efficient manner (98 : 2 dr and >82% yields). These β-aziridinyl-2-yl-β-hydroxy ketones were applied for the total synthesis of various alkaloids including (−)-epiallo-isomuscarine, the (2S,3R,5S)-enigmol analog, and epi-galantinic acid.

Highly Efficient and Stereoselective Mukaiyama Aldol Reaction with Chiral Aziridine-2-carboxaldehyde and Its Synthetic Applications

Nikhil Srivastava, Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, Yongin,17035, Korea, hjha@hufs.ac.kr

Abstract

We successfully synthesized a highly stereoselective β-aziridin-2-yl-β-hydroxy ketones by the Mukaiyama aldol reaction between optically pure 1-(α-methylbenzyl) aziridine-2-carboxaldehyde and various enol-silanes with $ZnCl_2$ via a chelation-controlled transition state in a highly efficient manner (98 : 2 *dr* and >82% yields). These β-aziridinyl-2-yl-β-hydroxy ketones were applied for the total synthesis of various alkaloids including (−)-*epiallo*-isomuscarine, the (2*S*,3*R*,5*S*)-enigmol analog, and *epi*-galantinic acid.

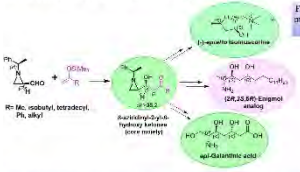


Figure : A Schematic Presentation of the Chelation-Controlled Transition state (TS) to yield the *erythro* isomer with the "*si*" face addition.

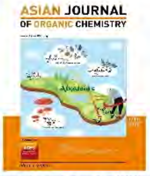
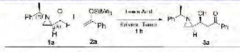


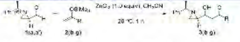
Table 1. Optimization of the Lewis acid-promoted Mukaiyama aldol reaction of chiral aziridine aldehyde **1a** with (trimethylsiloxy)styrene **2a** as a model substrate to obtain diastereoselective β-aziridin-2-yl)-β-hydroxy ketone **3a**.



Entry^a	Lewis acid^b	Equiv	Temp (°C)^c	Solvent	Yield (%)^d	dr of 3a (*E*:*Z*)^e
1	$BF_3{\cdot}OEt_2$	0.5	-78	CH_2Cl_2	15	>90:10
2	$BF_3{\cdot}OEt_2$	0.5	[illegible]	CH_2Cl_2	25	80:20
3	$BF_3{\cdot}OEt_2$	1.0	0	CH_2Cl_2	30	72:28
4	$BF_3{\cdot}OEt_2$	2.0	-78	CH_2Cl_2	[illegible]	[illegible]
5	$BF_3{\cdot}OEt_2$	2.0	0	CH_2Cl_2	[illegible]	[illegible]
6	$BF_3{\cdot}OEt_2$	2.5	0	1,4-dioxane	<10	-
7	$MgBr_2$	0.5	-78	CH_2Cl_2	NR	-
8	$MgBr_2$	0.5	-78	THF	NR	
9	$ZnCl_2$	0.5	-78	THF	NR	-
10	$ZnCl_2$	0.5	-78	EtOH	NR	
11	$ZnCl_2$	0.5	-78	CH_2Cl_2	25	>98:2
12	$ZnCl_2$	0.5	-78	CH_3CN	40	>98:2
13	$ZnCl_2$	1.0	-40	[illegible]	[illegible]	[illegible]
14	$ZnCl_2$	1.0	-20	CH_3CN	90	>98:2
15	$ZnCl_2$	1.0	23	CH_3CN	90	70:30

^{a}Reaction was performed at 0.5 mmol of compound 1a and compound 2a. ^{b}Lewis acid (1.0 equiv), ^{c}Temperature, ^{d}Isolated yield, ^{e}Diastereomeric ratio (*E*:*Z*) of product 3a.

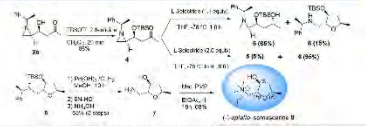
Table 2. Substrate scope of various enol silyl ethers 2 (b-g) to give β-(aziridin-2-yl)-β-hydroxy ketones 3 (b-g).



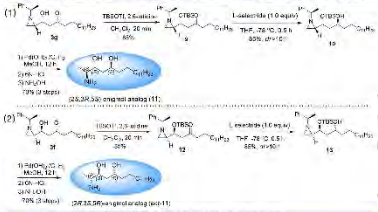
Entry	Aziridine-2-aldehyde (1a,a')^a	Silyl enol ether 2 (b-g)^a	Yield (%)^b 3 (b-g)	dr of 3 (b-g) (*E*/*Z*)^c
1	1a	2b	3b (80)	>95:5
2	1a	2c	3c (85)	>94:6
3	1a'	2d	3d (88)	>95:5
4	1a	2e	3e (85)	>97:3
5	1a'	2f	3f (80)	>96:4
6	1a'	2g	3g (82)	10:90

^{a}Reaction performed at 0.5 mmol of compound 1 and compound 2. ^{b}Isolated yield, ^{c}diastereomeric ratio (*E*/*Z*) of product 3 (b-g).

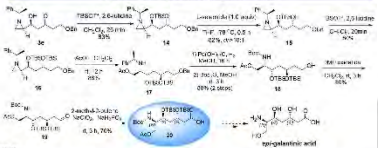
Forward Total Synthesis of 1-((2*R*,3*S*,5*R*)-3-hydroxy-5-methyltetrahydrofuran-2-yl)-*N*,*N*,*N*-trimethylmethanaminium iodide, (−)-*epiallo*-isomuscarine iodide.



Forward (1) Total Synthesis of (2*S*,3*R*,5*S*)-2-aminooctadecane-3,5-diol (11) an enigmol analog and (2) *ent*-(2*R*,3*S*,5*R*)-2-aminooctadecane-3,5-diol as an *ent*-(2*R*,3*S*,5*R*)-enigmol analog (*ent*-11).



Forward Total Synthesis of *epi*-galantinic acid



Reference

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4. Mao, H.; Jeong, H.; Yang, J.; Ha, H.-J.; Yang, J. W., *Chem. Eur. J.*, 2018, 24, 2370-2374.

Poster Presentation : **ORGN.P-444**

Organic Chemistry

Event Hall FRI 11:00~13:00

C2-Selective, Functional-Group-Divergent Amination of Pyrimidines by Enthalpy-Controlled Nucleophilic Functionalization

Hoonchul Choi, Dongwook Kim[1], Sukbok Chang[2,*]

Korea Advanced Institute of Science and Technology, Korea

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[2]*Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea*

Heteroaryl amines are prominent structural motif found in numerous bioactive molecules. In particular, 2-aminopyrimidines are an important class of molecular scaffolds in discovery chemistry, but a broadly applicable strategy for C2-selective amination of pyrimidines has been elusive to this date. Herein, we present a synthetic platform that enables site-selective C-H functionalization affording pyrimidinyl iminium salt intermediates, which subsequently allows transformations into various amines in situ. Mechanism-based reagent design facilitated the development of C2-selective amination of pyrimidines which have been previously elusive, but highly sought-after. Our method can be widely applied in the synthesis of pharmaceutically relevant heteroaryl amines.

Poster Presentation : **ORGN.P-445**

Organic Chemistry

Event Hall FRI 11:00~13:00

Copper-NHC Complexes as Catalysts for C-H Arylation of Aryloxazoles : Synthesis of Balsoxine, Texamine and Texaline

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Chemistry, Kyungpook National University, Korea

[1]*Eco-Friendly New Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

N-Heterocyclic carbens (NHCs) have played a significant role as ligands in the transition-metal catalytic reaction. Cu-NHC complex is one of these metal-NHC complexes, which has received much attention as an efficient catalyst for C-H activation reactions. Described here is the efficient C-H (het)arylation of aryloxazoles with (het)aryl iodides using a catalytic amount of Cu-NHC complex. This method was applicable to a broad range of substrates and the synthesis of balsoxine, texamine and texaline, known as the biologically active compounds.

Poster Presentation : **ORGN.P-446**

Organic Chemistry

Event Hall FRI 11:00~13:00

DNA-Compatible Synthesis of Imidazopyridine Derivatives using Groebke-Blackburn-Bienaymé Reaction

Yujin An, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

The DNA-encoded library (DEL), which is currently attracting attention in academia and the pharmaceutical industry, can link short DNA tags to small organic molecules to develop hundreds of thousands to billions of compounds and quickly discover new drugs. However, research to build a diverse and wide range of DELs is still urgent.In this study, the synthesis of imidazopyridine derivatives using the Groebke-Blackburn-Bienaymé (GBB) reaction, which is one of the multicomponent reactions for application to DEL, is to be described. First, the GBB reaction was optimized in off-DNA and aqueous solution conditions, and this was extended to on-DNA conditions. In addition, the Suzuki-Miyaura reaction, which is widely used for DEL synthesis, was added for library expansion. On-DNA synthesis results and directions for DEL construction will be described in detail.

Poster Presentation : **ORGN.P-447**

Organic Chemistry

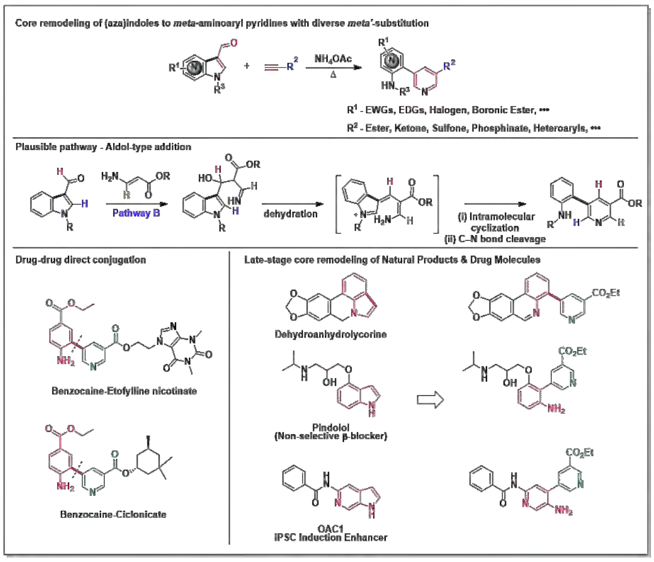
Event Hall FRI 11:00~13:00

Core Remodeling of (Aza)indoles to Novel *meta*-Aminoaryl Pyridine Structure for Direct Conjugation of Bioactive Pyridines and Anilines

Sihyeong Yi, Kannan Vaithegi, Ji Hyae Lee, Seung Bum Park*

Division of Chemistry, Seoul National University, Korea

Pyridine is a unique class of heterocycles that play an important role in biological systems. Highly potent as a bio-relevant privileged scaffold, pyridine is found in diverse biologically active drug small molecules and natural products. *meta*-Substituted pyridine, represented by niacin (or nicotinate), is a subclass of pyridines. However, it is hard to approach selectively *meta*-substituted pyridine with conventional methods. Bohlmann-Rahtz pyridine synthesis, one of the most widely used condensation-based synthetic method, can successfully generate *meta*-electron withdrawing group substituted pyridines with inevitable *ortho*-substitution.Here, we report a novel core remodeling method of (aza)indoles to generate *meta*-aminoaryl pyridines with diverse *meta*’-substitution without *ortho*-substitution. In this methodology terminal acetylenes are used as the source of *in situ* generated enamine species. A wide range of functional groups, including halogens and boronic esters, are tolerant to this methodology which differentiates from other cross-coupling strategies. By diversifying the terminal acetylenes resulted in diverse *meta*’-substitution including diverse keto analogous functional groups and even heteroaryls. By deuterium labeling experiment, aldol-type reaction mechanism was revealed. This methodology showed its synthetic power in late-stage conjugation of bioactive (hetero)arylamines with nicotinates and nicotinamides. Especially, the synthetic results for ester substitution, nicotinate analogues, were recently reported in Nat. Comm. 2020, *11*, 6308.


Core remodeling of (aza)indoles to meta-aminoaryl pyridines with diverse meta'-substitution
NH4OAc
Δ
R1 - EWGs, EDGs, Halogen, Boronic Ester, •••
R2 - Ester, Ketone, Sulfone, Phosphinate, Heteroaryls, •••
Plausible pathway - Aldol-type addition
Pathway B
dehydration
(i) Intramolecular cyclization
(ii) C–N bond cleavage
Drug-drug direct conjugation
Benzocaine-Etofylline nicotinate
Benzocaine-Ciclonicate
Late-stage core remodeling of Natural Products & Drug Molecules
Dehydroanhydrolycorine
Pindolol
(Non-selective β-blocker)
OAC1
iPSC Induction Enhancer

Poster Presentation : **ORGN.P-448**
Organic Chemistry
Event Hall FRI 11:00~13:00

Phenacyl Photoremovable Protecting Group Activated by Phenol

Ho Suk Shin, Bong Ser Park*

Department of Chemistry, Dongguk University, Korea

Phenacyl photoremovable protecting groups utilizing inter- and intramolecular electron transfer from phenol have been synthesized and studied. UV photolysis of the molecules results in the efficient release of benzoic acid. The photochemical reaction shows an interesting solvent effect, which in benzene reduction product is a major product but in protic solvents a coupling of phenacyl group and phenol occurs in major parts. Our product based studies and solvent isotope effect suggest that the reaction is assisted by hydrogen bond between the phenacyl esters and solvents. Photolysis of the phenacyl esters that contains a covalently linked phenol in protic solvents forms a new [3,3]paracyclophane whose structure was confirmed by X-ray crystallography. The [3,3]paracyclophane has a benzoyl moiety in which the carbonyl group in the short connecting bridge is twisted ca. 30 degrees away from the phenyl ring due to the rigid nature of the skeleton.

Poster Presentation : **ORGN.P-449**

Organic Chemistry

Event Hall FRI 11:00~13:00

Tin(II) Chloride-catalyzed Reductive Amination for Synthesis of Saturated *N*-Heterocycles from Dicarboxylic Acids

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

N-Heterocycle moieties such as pyrrolidine, piperidine, and azepane structures are considered as crucial building block motifs in organic chemistry. For this reason, discovering novel preparation method for *N*-heterocycles has attracted big interest of scientists. Besides, dicarboxylic acids are widely found and can be easily obtained. In this study, effective method for synthesizing saturated *N*-heterocycles from dicarboxylic acids and aryl amines is described. During the tests to find optimal condition, it was discovered that phenylsilane and tin(II) chloride could be used as a hydride source and a useful catalyst respectively to generate *N*-heterocycles from dicarboxylic acids. Reactions using phenylsilane and tin(II) chloride showed that various five-, six-, and seven-membered *N*-heterocycles were smoothly synthesized from succinic, glutaric, and adipic acids in high yields. This finding suggested that novel method can provide the efficient synthesis of a variety of valuable *N*-heterocycles.

Poster Presentation : **ORGN.P-450**

Organic Chemistry

Event Hall FRI 11:00~13:00

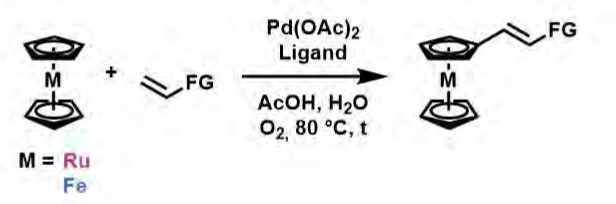
Alkenylation of Metallocenes via Palladium-Catalyzed C–H Functionalization

Sven florian Mueller, Jung Min Joo[1,*]

Department of Chemistry, Pusan National University, Germany

[1]*Department of Chemistry, Pusan National University, Korea*

A new catalytic system for the alkenylation of two metallocenes, ferrocene and ruthenocene, was developed. The choice of ligand, among other parameters, proved crucial in order to achieve the desired mono-alkenylation with a high degree of selectivity. The tolerance towards a wide array of functional groups on the olefin substrate was investigated and the supremacy of our ligand system over previously reported ones was demonstrated using kinetic experiments. Furthermore, insights into the reaction mechanism were gained by performing deuterium labelling experiments. In addition, the comparative reactivity of both metallocenes was examined during a competition experiment.



Poster Presentation : **ORGN.P-451**

Organic Chemistry

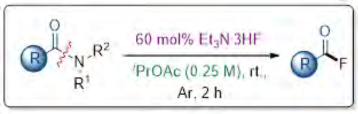
Event Hall FRI 11:00~13:00

Metal-free Synthesis of Acyl Fluorides from Amides via C-N Bond Cleavage

<u>Muhammad Aliyu Idris</u>, Karthik Rajan Rajamanickam[1], Jonghoon Oh[2], Sunwoo Lee[2,*]

Chemistry, Chonnam National University, Korea
[1]*CHEMISTRY, Chonnam National University, Korea*
[2]*Department of Chemistry, Chonnam National University, Korea*

Nowadays, the use of amides as an acyl or aryl source in cross-coupling reactions, leading to synthetically-valuable functional group inter-conversion of the amide bond is gaining huge attention. In this work, amides such as N-benzoylsaccharin, N,N-diBocbenzamide, and N-phenyl-N-tosylbenzamides reacted with $Et_3N.3HF$ to provide the corresponding acyl fluorides in good yields. The reaction was conducted under environmentally benign conditions using i-PrOAc as the solvent and a non-toxic fluorinating reagent. Moreover, the reaction was performed at room temperature and did not require a transition-metal catalyst or additives. The methodology showed functional group tolerance toward amines, alkoxy, halides, ketones, esters, and aldehydes.



Poster Presentation : **ORGN.P-452**

Organic Chemistry

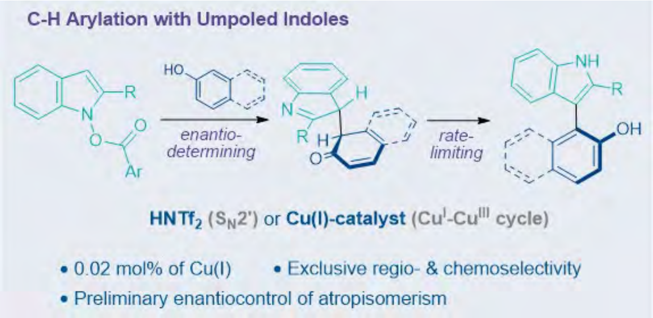
Event Hall FRI 11:00~13:00

Ortho-selective C–H arylation of phenols with *N*-carboxyindoles under Brønsted acid- or Cu(I)-catalysis

Nguyen Nguyen, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

The synthesis of bi(hetero)aryl compounds is an appealing topic due to their appearance in bioactive natural products, chiral auxiliaries and ligands.[1] However, control over chemo- and regioselectivity is a critical issue in the heterobiaryl synthesis via C–H oxidative coupling. To address this challenge, we developed a strategy for inverting the normal polarity of indoles in the heterobiaryl coupling reaction. Although the Cu(I)-catalyzed enantioselective alkylation of *N*-carboxyindoles was reported recently,[2] the development of C–H arylation protocol based on the *N*-hydroxyindole derivatives as umpoled coupling partner remains unexplored. With *N*-carboxyindoles as umpoled indoles, we demonstrated herein an exclusively *ortho*-selective coupling with phenols, employing a Brønsted acid- or Cu(I)-catalyst (as low as 0.01 mol%).[3] A range of phenols and *N*-carboxyindoles coupled with exceptional efficiency and selectivity at ambient temperature and the substrates bearing redox-active aryl halides (–Br and –I) smoothly coupled in an orthogonal manner. Notably, preliminary examples of atropselective heterobiaryl coupling have been achieved, based on a chiral disulfonimide or a Cu(I)/chiral bisphosphine catalytic system. The reaction was proposed to occur through S_N2' substitution or a Cu(I)–Cu(III) cycle, with Brønsted acid or Cu(I) catalysts, respectively.References:1. T. Wezeman, S. Bräse and K.-S. Masters, *Nat. Prod. Rep.*, **2015**, *32*, 6.2. Y. Ye, S.-T. Kim, J. Jeong, M.-H. Baik and S. L. Buchwald, *J. Am. Chem. Soc.*, **2019**, *141*, 3901.3. N. H. Nguyen, S. M. Oh, C. Park, S. Shin, *Chem. Sci.*, **2022**, *13*, 1169.


C-H Arylation with Umpoled Indoles
R
N
O
O
Ar
HO
enantio-determining
N
R
H
H
O
rate-limiting
NH
R
OH
HNTf$_2$ (S$_N$2') or Cu(I)-catalyst (Cu^I-Cu^{III} cycle)
• 0.02 mol% of Cu(I)
• Exclusive regio- & chemoselectivity
• Preliminary enantiocontrol of atropisomerism

Poster Presentation : **ORGN.P-453**

Organic Chemistry

Event Hall FRI 11:00~13:00

Okadaic Acid Detecion Using the Fluorometric Quenching Assay with OA-Specific Bioreceptors *via* Phage Display

So Yeon Kweon, Sunghyun Kim[1], Tae Jung Park*

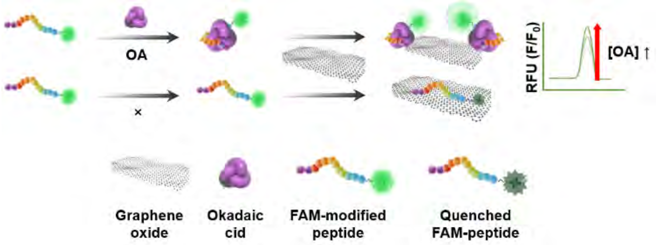
Department of Chemistry, Chung-Ang University, Korea

[1]*nanobio-chemistry, Chung-Ang University, Korea*

As marine toxins in seafood arouse severe health risks to public health, most countries have urged to regulate and monitor the maximum content of toxins in marine products. Okadaic acid (OA) causes diarrhea by stimulating the phosphorylation of proteins that controls sodium secretion by intestinal cells, resulting in a massive loss of fluids. In consequence, the consumption of OA-contaminated shellfish induces various severe gastrointestinal disorders such as vomiting, nausea, and diarrhea. Internationally accepted method for their detection is HPLC-fluorescence detection method. While the method offers better sensitivity, it requires lengthy procedures and complex data interpretation. Herein, we have developed okadaic acid-specific bindable bioreceptors through the phage display technology for overcoming the above problems. For this technique, we present the haptenization of okadaic acid by conjugating with bovine serum albumin (BSA). To effectively immobilize the OA on the BSA, DCC/NHS crosslinking method was used. The discovered bioreceptor was then applied for the fluorescence detection system with graphene oxide as a quencher.

Funding : This research was funded by Ministry of Food and Drug Safety grant number 20163MFDS641.

Acknowledgments : This research was supported by a grant (20163MFDS641) from Ministry of Food and Drug Safety in 2022.


OA
×
RFU (F/F$_0$)
[OA] ↑
Graphene oxide
Okadaic cid
FAM-modified peptide
Quenched FAM-peptide

Poster Presentation : **ORGN.P-454**

Organic Chemistry

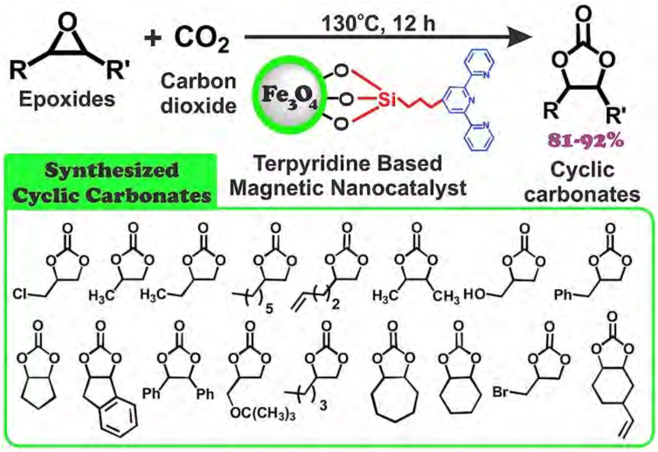
Event Hall FRI 11:00~13:00

Terpyridine-Pr-Fe_3O_4@boehmite nanoparticles; a novel and highly effective magnetic nanocatalyst for preparation of cyclic carbonates from carbon dioxide and epoxides under solventless conditions

Faisal Muhammad

Organic and medicinal chemistry, University of Science & Technology, Korea

In this research work, moisture- and air-stable terpyridine-mediated magnetic boehmite (terpyridine-Pr-Fe_3O_4@boehmite) nanocatalyst was fabricated and applied for the synthesis of cyclic carbonates. The nanocatalyst was constructed by very simple process using commercially available starting materials and fully characterized through various techniques including FT-IR, VSM, SEM, TGA, N_2 adsorption-desorption isotherm, elemental analysis and leaching test. The characterizations results suggested the superparamagnetic nature of the Fe3O4 nucleus encapsulated by a boehmite nanoparticles shell. Further, nanoparticles could be used safety in organic reactions owing to large thermal stability of around 300 °C and can be applicable under strong acidic and basic reaction conditions. Additionally, the nanoparticles were of hexagonal like shape, uniformly distributed and much uniform in size, with an average size about 50 nm. Terpyridine-Pr-Fe_3O_4@boehmite nanoparticles were applied as nanocatalyst for the synthesis of cyclic carbonates form the cycloaddition coupling reaction of CO_2 with epoxides under solventless conditions. The cost-effective nanocatalyst tolerated a broad variety of functional groups. The one-pot and practical procedure offers numerous benefits such as good to excellent yields, environment-friendliness, low catalyst loading and operational simplicity. Additionally, the durability of catalyst was investigated and observed that the catalyst is stable under the reaction conditions and could be isolated easily from the reaction content by using a bar magnet and reused for several consecutive cycles without any important loss of catalytic potency.


R
R'
Epoxides
+ CO2
Carbon dioxide
130°C, 12 h
Fe3O4
Si
N
Terpyridine Based Magnetic Nanocatalyst
O
O
O
R
R'
81-92%
Cyclic carbonates
Synthesized Cyclic Carbonates
Cl
H3C
H3C
5
2
H3C
CH3
HO
Ph
Ph
Ph
OC(CH3)3
3
Br

Poster Presentation : **ORGN.P-455**
Organic Chemistry
Event Hall FRI 11:00~13:00

Chiral Lewis Acid Catalyzed Enantioselective Addition of α-Aminoalkyl Radical Initiated by Visible Light

Soo Min Cho, Shinyeong Han, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Photoredox catalysis induced by visible light have attracted interest because radical makes it possible to develop new reaction pathways that are difficult with previous catalysis. Using photoredox catalysis, the tertiary alcohol product, which is difficult to synthesize because of its steric hindrance, could be easily produced through radical addition to ketone compounds. Because the tertiary alcohol scaffold is prevalent in organic molecules, it is important to develop the efficient synthetic route for tertiary alcohol. Until now, the only a few examples of enantioselective photoredox reactions using ketones are reported.[1] In this research, we developed an enantioselective addition of *α*–aminoalkyl radical, which is induced by visible light, to acetophenone derivatives catalyzed by chiral oxazaborolidinium ion (COBI) as Lewis acid catalyst. Using this method, highly optically active *β*-amino tertiary alcohols were generated in high yields (up to 88%) with excellent enantioselectivities (up to 98%).**References**[1] (a) C. Wang, J. Qin, X. Shen, R. Riedel, K. Harms, E. Meggers *Angew. Chem. Int. Ed.* **2016**, *55*, 685. (b) J. Ma, K. Harms, E. Meggers *Chem. Commun.* **2016**, *52*, 10183. (c) Y. Liu, X. Liu, J. Li, X. Zhao, B. Qiao, Z. Jiang *Chem. Sci.* **2018**, *9*, 8094. (d) K. Cao, S. M. Tan, R. Lee, S. Yang, H. Jia, X. Zhao, B. Qiao, Z. Jiang *J. Am. Chem. Soc.* **2019**, *141*, 5437.[2] J. Y. Kim, Y. S. Lee, Y. Choi, D. H. Ryu *ACS Catal.* **2020**, *10*, 10585.

Poster Presentation : **ORGN.P-456**

Organic Chemistry

Event Hall FRI 11:00~13:00

Palladium loaded a nitrogen rich imine-linked covalent organic framework as a heterogenous catalyst for Suzuki coupling

Ju gyeong Jeong[*], Dong Wook Kim[1,*]

Chemistry, Inha University, Korea

[1]*Department of Chemistry, Inha University, Korea*

TpTta COF is one of the imine-linked covalent organic frameworks, which are synthesized through Schiff condensation reaction between 1,3,5-triformyl phloroglucinol (Tp) and 1,3,5-tris-(4-aminophenyl)triazine(Tta) under solvothermal condition. TpTta COFs can be applied to various fields because of their superior characteristics including high crystallinity, porous structure, functionality, metal-free, chemical stability, luminescent properties. In Particular, due to its excellent chemical stability and high nitrogen functionality, $Pd(OAc)_2$ was easily loaded into TpTta COF structures and utilized as a heterogeneous catalyst. Pd loaded TpTta COF as a catalyst was tested for a Suzuki coupling reaction of aryl boronic acid and aryl halides. A Suzuki coupling reaction using this Pd loaded heterogenous catalyst (0.5mol% of palladium) provided the wanted product in 98.0% yield. In addition, this catalyst can be recycled without any noticeable loss of catalytic activity.

Poster Presentation : **ORGN.P-457**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of azaindole derivatives as a radiopharmaceuticals for tau protein targeting PET imaging probe.

Su Jin Park*, Dong Wook Kim*

Department of Chemistry, Inha University, Korea

Tau protein is one of the neuropathological features of Alzheimer's patients and is considered be an important cause of dementia. We can understand more about dementia-related diseases by making a PET imaging probe targeting the tau protein for understanding the mechanism of progression of Alzheimer's disease and for diagnosis of patients. Therefore, for the preparing of azaindole derivatives we have introduced a fluorine-prosthetic group into azaindole compounds at 6 and 7 position. We synthesized 16 azaindole derivatives and [18]F was labeled on two compounds having a fluoro-prosthetic group introduced at the 7 position of azaindole among the synthesized compounds to measure binding affinity to KR201. The synthesized azaindole derivatives were carried out to autoradiography through in-vitro tests on the hippocampus and frontal cortex in the brain tissue of Alzheimer's disease patients. Therefore, it will be a good starting point for future in vivo tests and development of more tau tracers.

Poster Presentation : **ORGN.P-458**
Organic Chemistry
Event Hall FRI 11:00~13:00

Sustainable Ir(triscarbene)-Catalyzed Reaction : Synthesis of GVL and β-alkylated alcohols

Mi-hyun Lee, Kihyuk Sung[1], Hye-Young Jang[2,*]

Department of Energy System Research, Ajou University, Korea
[1]*Department of Energy Systems Research, Ajou University, Korea*
[2]*Department of Chemistry, Ajou University, Korea*

The organometallic catalyst has contributed to sustainable chemistry by upcycling biomass and replacing traditional methods employing petroleum. Transition metal-catalyzed transfer hydrogenation converted biomass-derived levulinic acid to industrially useful gamma-valerolacton(GVL). GVL is used as a solvent in various industries due to its characteristics such as low toxicity and low volatility. In addition, it has a higher energy density than ethanol, so it can be used directly as a fuel or fuel additives. Transition metal-catalyzed cross-coupling of biomass-derived alcohols can be used for the synthesis of high molecular weight branched alcohols, which can be applied to detergents and lubricants. In this study, we synthesized iridium(I) complexes using NHC ligands, which were used to enhance the stability and efficiency of the catalyst. By utilizing iridium(I) catalysts, biomass-derived levulinic acid was converted to GVL using glycerol as a hydrogen source. Structurally diverse alcohols were also synthesized through the condensation of alcohols in the presence of the same catalyst.

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Poster Presentation : **ORGN.P-459**

Organic Chemistry

Event Hall FRI 11:00~13:00

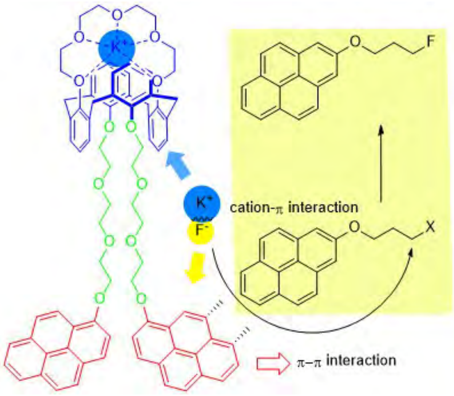
Pyrene-substituted bis-triethylene glycolic crown-5-calix[4]arene as a π-π interaction promoted phase transfer catalyst for nucleophilic fluorinations

Geunhyuck Bak[*], **Kim Yong Kwon**[1], **Dong Wook Kim**[*]

Department of Chemistry, Inha University, Korea

[1]*Dept. of chemistry, Inha University, Korea*

We designed and synthesized a pyrene-substituted bis-triethylene glycolic crown-5-calix[4]arene (Pyrene-BTC5A) as phase transfer catalysts(PTC) for the S_N2 fluorination using potassium fluoride. Crown-5-calix[4]arene holds potassium ions, poly ether acts as a Lewis base, and terminal pyrene groups brings the starting material closer to the fluorine ion through π-π interaction and proximity effect. This catalyst showed good performance in nucleophilic fluorinations through in π-π interaction. Through this, tested for faster nucleophilic fluorination reaction by applying it to a precursor with π electrons rich aromatic compound. It was confirmed that the material with π electrons rich aromatic compound such as pyrene had a faster nucleophilic fluorine reaction rate than the material with poor π electrons. In addition, the reaction rate was tested under various reaction conditions. Experiments using three substrates, pyrene, naphthyl, and t-phenyl, confirmed the effect of π-π interaction. In this result, pyrene substrate had the fastest reaction rate that is considered a proximity effect.



Poster Presentation : **ORGN.P-460**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Confirmation of Hemilabile Polydentate Ligands

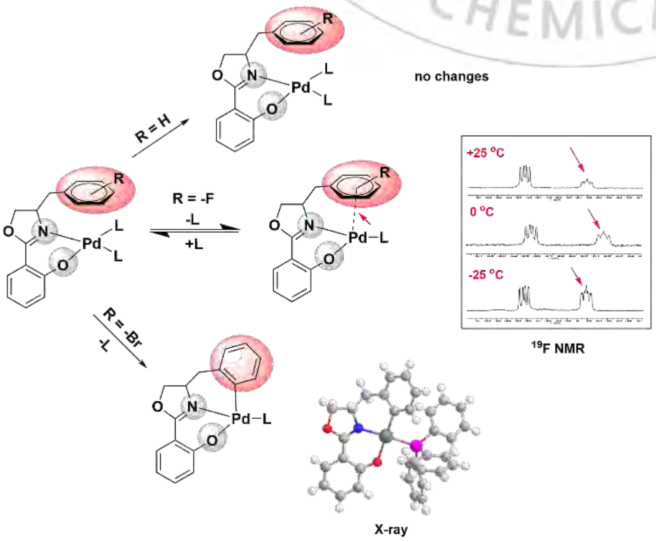
On-Yu Kang, Guldana Issabayeva[1], Hyun Jiyoung[2], Seong Jun Park[2,*], Do Hyun Ryu[*], Hwan Jung Lim[2,*]

Department of Chemistry, Sungkyunkwan University, Korea

[1]*Department of Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea*

[2]*Data Convergence Drug Discovery Research Center, Korea Research Institute of Chemical Technology, Korea*

The fluxional behavior of a hemilabile moiety provides a vacant coordination site at the transition metal (TM) center for a substrate to bind to during the catalytic cycle. Based on an interest in the fluxional behavior of π-electron-containing systems, we studied new a palladium (II) complex bearing polydentate mono(oxazoline) O,N,$CH_2η^6$-Ar ligands (Ar= C_6HF_4, C_6F_5, C_6H_4Br, and C_6H_5) with fluorinated arene as a labile moiety. The fluorinated arene was assumed to coordinate to palladium (II) in an $η^6$-manner. The presence of fluorine substituents on the fluxional moiety enhanced the hemilability of the aromatic ring at lower temperatures. Fluorine NMR studies showed the formation of the complex.



Poster Presentation : **ORGN.P-461**

Organic Chemistry

Event Hall FRI 11:00~13:00

Asymmetric Michael Addition in Water Using New Proline-Derived Organocatalysts

Jin Won Lee, Do Hyun Ryu[*]

Department of Chemistry, Sungkyunkwan University, Korea

Using water as a solvent is environment friendly, non-flammable, less expensive, non-toxic and safe compared to the organic solvents. Therefore, developing organocatalyst that act on aqueous medium is important for asymmetric catalytic green reaction to mimic the action of enzymes in nature as well as to achieve high reactivity and stereoselectivity. Herein, we report new proline derived secondary amine organocatalysts based on efficient chiral scaffold to examine the performance in Michael addition between nitroolefins and carbonyl compounds that enforced by hydrophobic amplification in aqueous medium. Furthermore, we also demonstrated that proper relative stereochemistry at C_6 in catalyst plays a key role in successful catalysis.

Poster Presentation : **ORGN.P-462**

Organic Chemistry

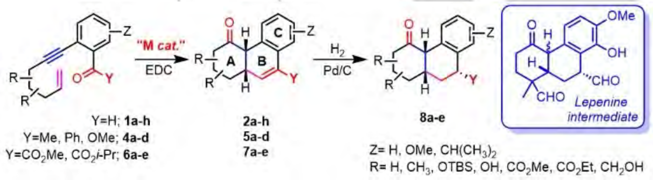
Event Hall FRI 11:00~13:00

Synthesis of [6,6,6]-tricyclic compounds from enyne carbonyl via copper-catalyzed cyclization

<u>Juyeon Kang</u>, Juhui Lee, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

Synthesis of natural product Lepenine intermediate is important because it exhibits various pharmacological properties owing to its unique structural characteristics. Intramolecular cycloaddition is an efficient method for synthesizing [6,6,6]-tricyclic compounds and has been conducted for many years. We performed copper-catalyzed cyclization from enyne-carbonyl substrates containing H, Me, Ph, OMe, CO2Me, and CO2i-Pr (Y groups) of aryl moieties.



Poster Presentation : **ORGN.P-463**

Organic Chemistry

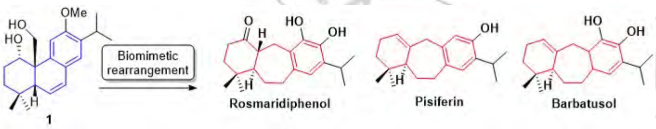
Event Hall FRI 11:00~13:00

Total synthesis of Icetexane diterpenoids via biomimetic rearrangement

Le Thuy Quynh, Sunmin Kwon[1], Chang Ho Oh[2,*]

Chemistry department, Hanyang University, Korea
[1]*Hanyang University, Korea*
[2]*Department of Chemistry, Hanyang University, Korea*

The abietanes and icetexanes are diterpenoid natural products that have been isolated from Salvia plants. The common core skeleton of abitane is a [6-6-6] tricyclic framework. Biosynthetically, 9(10→20)-abeo-abietane is the formal name of the [6-7-6] fused icetexane skeleton which arises via a natural rearrangement of the corresponding [6-6-6] fused abietane diterpenoids Herein, we report the rearrangement of abitane core 1 with trifluoromethanesulfonic anhydride in pyridine afforded the icetexane core, which was key intermediate for the total synthesis of structurally intriguing and biologically active compounds Barbatusol, Rosmaridiphenol and Pisiferin



Poster Presentation : **ORGN.P-464**

Organic Chemistry

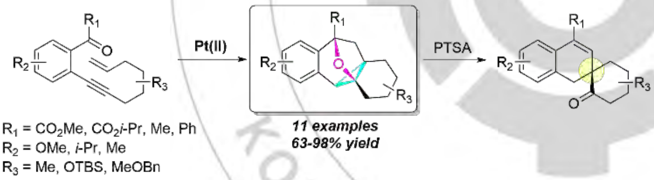
Event Hall FRI 11:00~13:00

Synthesis of cyclopropanes with oxa-bridge via [3+2] cyclization of Pt-carbenes complex : Extended substrates from enynal to enynone

Juhui Lee, Chang Ho Oh[*]

Department of Chemistry, Hanyang University, Korea

We synthesized cyclopropanes having an Oxa-bridge. Previously our group has carried out platinum-catalyzed reactions using only aldehydes. In this work, we synthesized various tricyclic compounds using wide substrates with acetyl and ester groups. Then heated under p-TsOH and benzene, a spiro compound could be easily obtained with good stereoselectivity and high yields.



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Poster Presentation : **ORGN.P-465**

Organic Chemistry

Event Hall FRI 11:00~13:00

DDQ-Catalyzed trifluoromethylation and fluorocarbamoylation using the Langlois reagent

Hui jeong Cho, Sun-Joon Min[1,*]

chemistry, Hanyang University, Korea
[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Fluorination has become an important synthetic method in modifying and controlling properties of compounds. In particular, fluorine-containing drugs are increasing in drug discovery because fluorine atom can significantly influence drug metabolism, lipophilicity, metabolic stability, membrane permeability and bioavailability. In this regards, development of new fluorination strategies is required for installation of fluorine atom on the specific site of molecules.In this study, we describe a direct C-H trifluoromethylation of arenes using a readily available trimethylating reagent, sodium trifluoromethanesulfinate (CF_3SO2Na) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) as a photoredox organocatalyst. The reaction of electron-rich arenes in the presence of DDQ under blue light irradiation afforded the desired trifluoromethylated compounds in good yields. Alternatively, the reaction of secondary amines under the same condition in the presence of oxygen produced carbamoyl fluoride efficiently through carbonyl fluoride intermediate.Our effort to investigate substrate scope and reaction mechanisms in both transformations will be provided in this presentation.

Poster Presentation : **ORGN.P-466**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Chiral *β*-Keto Ester with All-carbon Quaternary Stereocenter Catalyzed by Chiral Lewis Catalysts

Hye-Min Jeong, Do Hyun Ryu[*]

Department of Chemistry, Sungkyunkwan University, Korea

The synthesis of molecules with all-carbon quaternary stereocenters is one of the most challenging topics in current organic chemistry. In many cases, transition metal catalysis has been used in the construction of chiral quaternary carbon, but this method has a limitation of costs and toxicity. However, only a few enantioselective reactions using organocatalyst to generate acyclic all-carbon quaternary stereocenter having 3 carbonyl groups were reported. In this research, we developed the method for synthesis of chiral acyclic *α*-quaternary-*β*-keto esters with aldehyde groups through the reaction of diazo ester with aldehyde compounds in the presence of chiral oxazaborolidinium ion (COBI) as Lewis acid catalysts. Using this methodology, the highly optically active *β*-keto ester having *α*-quaternary carbon centers were afforded in excellent yield (up to 97%) with excellent enantioselectivities (up to 98% ee). *β*-Keto esters are important compound in synthetic chemistry because it contains both electrophilic and nucleophilic sites. They often constitute a core building block in complex medicinal compounds.

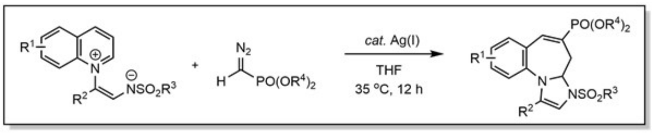
Poster Presentation : **ORGN.P-467**
Organic Chemistry
Event Hall FRI 11:00~13:00

Catalytic Dearomative Synthesis of Multi-Fused Azepines via Regioselective Ring-Expansion of Heteroarenes

Sekwang Baek, Hyundug Jen[1], Eun Jeong Yoo[2,*]

Chemisty, Kyung Hee University, Korea
[1]chemistry, Kyung Hee University, Korea
[2]Department of Applied Chemistry, Kyung Hee University, Korea

Since medium-sized N-heterocyclic scaffolds are prevalent in natural products, and biologically active molecules, their synthesis has attracted attention in various fields of chemistry. Among them, seven-membered azepines and diazepines are some of the most significant pharmacophores exhibiting diverse biological activities. Azepine derivatives, which are core structures of market drugs such as Benazepril, Mianserin, and Tolvaptan, have been prepared through conventional synthetic approaches, electrocyclizations, higher-order cycloadditions, and cross-coupling reactions.Our group has developed synthetic methods of N-aromatic zwitterions, which are site-switchable reagents for the construction of diverse N-heterocycles. Although N-aromatic zwitterions are practical and readily available starting materials, they have structural limitations that furnish cyclic products, inevitably fused with six-membered piperidine scaffolds. To overcome such shortcomings, we envisioned a cascade reaction using N-aromatic zwitterion, a formation of a strained small-ring followed by its expansion, to construct medium-sized N-heterocycles. In this presentation, we discuss synthetic methods for the construction of azepine derivatives through cycloadditive ring-expansions of N-aromatic zwitterions. It has been revealed that diazo acetates and diazo methylphosphonates are suitable to undergo cyclopropanations of N-aromatic zwitterions in the presence of a silver catalyst to provide the cyclopropane-fused intermediates, which are further expanded into desired azepines. The developed cycloadditive expansion reaction has been characterized by broad substrate scope, mild reaction conditions, easy scale-up reactivity, and easy synthetic applicability.



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Poster Presentation : **ORGN.P-468**

Organic Chemistry

Event Hall FRI 11:00~13:00

Asymmetric Synthesis of 2-Pyrazolines via Catalytic Enantioselective 1,3-Dipolar Cycloaddition

Terim Seo, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Chiral nitrogen-containing heterocycles, especially pyrazolines, are easily found in various natural products and pharmaceuticals.1) Because of their structural importance, asymmetric synthesis of pyrazolines has been investigated using several ways. Among these methods, catalytic 1,3-dipolar cycloaddition is one of the most efficient approaches for the enantioselective synthesis of pyrazolines.2) Herein, our group successfully synthesized enantio-enriched 2-pyrazolines in high to excellent yields (up to 99%) and enantioselectivities (up to >99%) via enantioselective 1,3-dipolar cycloadditions of *α*, *β*-unsaturated esters and diazo compounds catalyzed by chiral oxazaborolidinium ion (COBI) catalyst.References1. Remen L.; Benzençon O.; Simons L.; Gaston R.; Downing D.; Gatfield J.; Roch C.; Kessler M.; Mosbacher J.; Pfeifer T.; Grisostomi C.; Rey M.; Ertel E. A.; Moon R. *J. Med. Chem.* **2016**, *59*, 8398-84112. (a) Gao L.; Hwang G.-S.; Lee M. Y.; Ryu D. H. *Chem. Commun.* **2009**, *36*, 5460-5462; (b) Lee S. I.; Kim K. E.; Hwang G.-S.; Ryu D. H. *Org. Biomol. Chem.* **2015**, *13*, 2745-2749

Poster Presentation : **ORGN.P-469**

Organic Chemistry

Event Hall FRI 11:00~13:00

KO*t*-Bu catalyzed aza-Michael reaction of enones with pyrazoles

Subin Yoon, Yunmi Lee[1,*]

Chemistry, Kwangwoon University, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*

The formation of carbon-nitrogen bonds is very important in the construction of natural products, therapeutic agents and functional substances. Aza-Michael addition is one of the simplest and atomically economical processes for adding nucleophilic amines to electron deficient alkenes. In general, aza-Michael addition was carried out under strong acid or strong base conditions with high reaction temperature and long reaction time. In addition, it has been reported that aza-Michael addition can proceed efficiently and under mild conditions using a transition metal catalyst. In this study, a method for synthesizing β-pyrazolyl ketone by adding pyrazole to a cyclic enone with a low reaction temperature and relatively short reaction time using a base catalyst without using a transition metal catalyst is introduced. Considering the significance and challenges of the construction of *N*-substituted carbon quaternary centers, we pursued the exploration of an efficient and mild base-catalyzed aza-Michael addition to trisubstituted cyclic enones. The use of a readily available and inexpensive KO*t*-Bu catalyzed the addition of pyrazoles to trisubstituted cyclic enones, affording a variety of β-pyrazolyl ketones in high yields.

Poster Presentation : **ORGN.P-470**

Organic Chemistry

Event Hall FRI 11:00~13:00

Acid-Catalyzed Hydrolysis and Intramolecular Cyclization of *N*-Cyano Sulfoximines for the Synthesis of Thiadiazine 1-Oxides

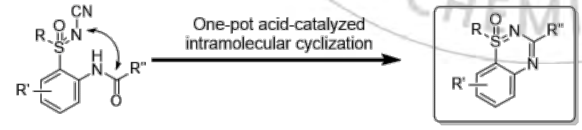
In Seok Oh, Eunsil Kim[1], Yeji Seo[2], Hyun Jiyoung, Hwan Jung Lim[*], Duck-Hyung Lee[1,*], Seong Jun Park[*]

Data Convergence Drug Discovery Research Center, Korea Research Institute of Chemical Technology, Korea

[1]*Department of Chemistry, Sogang University, Korea*

[2]*Department of Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea*

Here, we present a novel method for the practical synthesis of thiadiazine 1-oxides **10**. To prepare the desired thiadiazine 1-oxides **10**, the novel synthethic method of an intramolecular cyclization with 2-*N*-cyano-sulfonimidoyl amides **9** was successfully developed. One-pot acid-induced hydrolysis of the cyano group and the intramolecular cyclocondensation has provided a various heterocyclic compounds. The crystal structures of *N*-urea sulfoximine **11** and thiadiazine 1-oxide **10i** have been determined using X-ray crystallography.



9
N-Cyano sulfoximines

10
Thiadiazine 1-oxide

- Metal-free one-pot intramolecular cyclization of 2-*N*-cyano-sulfonimidoyl amides 9
- Simple raction, covenient method, and broad substrate scopes

Poster Presentation : **ORGN.P-471**

Organic Chemistry

Event Hall FRI 11:00~13:00

Aldehyde *N,N*-dimethylhydrazone-based fluorescent substrate for the peroxidase-mediated assays

Soyeon Yoo, Min Su Han[1,*]

Brain Science Institute, Korea Institute of Science and Technology, Korea

[1]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

This study details the development of a new fluorescent peroxidase substrate for H_2O_2 detection based on peroxidase activity. Previously developed peroxidase substrates have problems associated with poor light stability, over-oxidation by excess H_2O_2, and limited workable pH. Therefore, a fluorescent peroxidase substrate that retains high stability to the surrounding environment such as light and acid would be desirable. Herein, we devised 2-((6-methoxynaphthalen-2-yl)methylene)-1,1-dimethylhydrazine (**MNDH**) as the fluorescent peroxidase substrate based on an oxidative cleavage reaction of aldehyde N,N-dimethylhydrazone by horseradish peroxidase (HRP) and H_2O_2. The **MNDH**/HRP system enabled quantitative H_2O_2 detection through an increase in fluorescence according to the concentration of H_2O_2 in a wide pH range from acidic to neutral. **MNDH** was very stable to ambient light and heat and retained a quantitative fluorescence signal even in the presence of an excess of H_2O_2. In addition, the **MNDH**-based enzyme cascade assay system quantitatively detected glucose levels in human serum. Furthermore, the strategy of using **MNDH** can be expanded to detect various analytes associated with hydrogen peroxide.

Poster Presentation : **ORGN.P-472**

Organic Chemistry

Event Hall FRI 11:00~13:00

Coupling of amide and sodium azide for the synthesis of acyl azide, symmetrical urea and iminophosphorane

Joseph Devaneyan, Hyemin Kang, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Amide functionality has been regarded as a less reactive carbonyl group in acyl substitution reactions due to the high stability of acyl C-N bond by the resonance effect. In this work, Electronically and rotationally active amides such as N-Trifluoromethansulfonyl, N-Mesityl N-Phenylbenzamides, N-Benzyl-N-tosylbenzamide, N,N-DiBoc protected benzamide and N-benzoyl saccharin has been used to synthesis of acyl azides and keto-stablized iminophosphoranes through the activation of amide C-N bond cleavage at room temperature and in warm condition undergoes Curtis rearrangement and forms symmetrical urea. It's noteworthy that no additives and metal catalyst has been performed.

Poster Presentation : **ORGN.P-473**

Organic Chemistry

Event Hall FRI 11:00~13:00

Selective Eradication of Bacteria by ROS Reactivity Differences

Hee Jeong Kim, Juyoung Yoon*

Chemistry & Nanoscience, Ewha Womans University, Korea

Photodynamic therapy(PDT) is attracting a lot of attention as a major research field. Using the significant feature that reactive oxygen species(ROS) are generated after light irradiation, PDT is applied in various ways such as anti-tumor and antibacterial treatment. Although various methods are being attempted to improve the efficiency of PDT, more fundamental mechanisms of the series of PDT processes are still needed to be revealed. In this study, our group synthesized two photosensitizers which are capable of generating singlet oxygen and superoxide radical anion, respectively to determine whether different reactive oxygen species can actually show a difference in antibacterial effect. In the *in vitro* experiment, it was confirmed that the two types of photosensitizers generated different kinds of ROS while the light is being irradiated. Interestingly, when PDT efficacy was tested in bacterial experiments using gram bacteria, the types of bacteria that two fluorophores can kill were different. Not only these findings, the mechanism of how ROS can exhibit toxicity in bacteria was observed in detail through a confocal laser scanning microscope(CLSM). As a result, in this study, it was obviously confirmed that the control of radical generation in PDT can selectively kill certain bacteria, suggesting that fundamental molecular design is still very important to efficiently control PDT efficacy.

Poster Presentation : **ORGN.P-474**

Organic Chemistry

Event Hall FRI 11:00~13:00

Utilization of N-Silyl Enamines from Borane-Catalyzed Hydrosilylation of Conjugated Nitriles for Formamidine and Ester Synthesis

Vinh Do cao, **Seewon Joung***

Department of Chemistry, Inha University, Korea

In recent research, we have developed a synthetic strategy to furnish Z-amidines from cyclic N-silyl enamines and organic azides via [3+2] cycloaddition following the rearrangement pathway. In this study, we have chosen the optimal conditions to obtain linear N-silyl enamines from borane-catalyzed hydrosilylation of conjugated nitriles. These linear N-silyl enamines also underwent [3+2] cycloaddition with organic azides, but triazoline intermediate occurred a different rearrangement pathway. With different features, we have developed a synthetic route to produce E-formamidines and utilized the co-products, being diazo alkanes, to produce ester with simple and mild condition.

Poster Presentation : **ORGN.P-475**

Organic Chemistry

Event Hall FRI 11:00~13:00

DNA-Compatible Mannich and Suzuki-Miyaura Reactions

Danila Ryzhikh, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

Since the invention of the DNA-encoded library (DEL) synthesis, the speed and efficiency of the drug discovery, especially in the early stages, increased significantly. Nowadays, almost every major pharmaceutical company utilizes this method as a core platform for finding and identification of medicinal substances. The main idea of the DEL technology is to combine combinatorial organic synthesis and DNA chemistry to produce the library of the unprecedented amount of small molecules with the unique DNA "barcode" for each molecule.There are plenty of named organic reactions that have been applied to DEL, however, reactions that have not yet been applied predominate. Among those reactions, the Mannich reaction is an interesting one. Mannich bases, the end products of the Mannich reaction, are already noticed as biologically active compounds possessing a wide range of activities such as anti-bacterial, anti-inflammatory, analgesic, etc. The importance of this reaction cannot be overestimated. Yet the investigations of the treating agents, containing the Mannich base within its structure, were narrowly focused on specific structures. Even though Suzuki-Miyaura cross-coupling has been widely studied in frames of DEL, the simultaneous application of Mannich and Suzuki reactions has still not been considered. We are applying both reactions mentioned above to the DEL design. This whole work was divided into two major parts: 1) Off-DNA, where the reactivity was estimated without the presence of the nucleotide chain; and 2) On-DNA, where the optimal conditions of the on-DNA reactions are evaluated. Therefore, the robust and efficient synthetic method for the DEL production, utilizing Mannich and Suzuki-Miyaura reactions, will be proposed.

Poster Presentation : **ORGN.P-476**

Organic Chemistry

Event Hall FRI 11:00~13:00

Simple Molecular Design Method of Advanced Thiocarbonyl-base Photosensitizers for Photodynamic Therapy

Moonyeon Cho, Sungnam Park[1,*], Juyoung Yoon[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Department of Chemistry, Korea University, Korea*

Photodynamic therapy (PDT) is a medical technique to treat various types of cancers and other disease. For PDT, three essential components are needed: a light-activated agent (photosensitizer, PS), light and oxygen. As an effective heavy-atom-free photosensitizer (PS), sulfur-substituted carbonyl fluorophores are well known due to their prominent phototherapeutic properties. However, mostly thiocarbonyl-based PSs are non-emissive in the solution and restricted state, so it's biomedical application are obstructed. In this study, we synthesized the CMS series and through the work we mainly report two things. First, sulfur-substituted coumarin shows aggregation-induced emission (AIE) which can be the key to solve the main problems thiocarbonyl-based PSs have. Second, the mitochondrial-targeting ability of coumarin fluorophores were enhanced by introducing a strong electron-withdrawing trifluoromethyl (CF3) group. The constructed agent CMS-2, consequently exhibited better PDT efficiency than commercial PS under green light irradiation. This project may provide a new perspective toward molecular design of next-generation thiobase-based PSs that have conspicuous cancer targeting ability.

Poster Presentation : **ORGN.P-477**

Organic Chemistry

Event Hall FRI 11:00~13:00

Stereoselective Synthesis of Benzo[*a*]quinolizidines via Aerobic DDQ-catalyzed Allylation

Sun Hwa Jung, Sun-Joon Min[1,*]

Department of Applied chemistry, Hanyang University, Korea

[1] *Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Tricyclic benzo[*a*]quinolizine ring system, a common structural motif in alkaloids, is found in various biologically active natural products and pharmacologically useful compounds. Due to the biological importance of benzo[*a*]quinolizidine analogues, many synthetic approaches towards this tricyclic structure have been developed.Recently, our research has focused on the synthesis of azacyclic compounds using DDQ-mediated Mannich type cyclization. To improve our strategy in the synthesis of azacycles, we planned a new synthetic process to construct benzo[*a*]quinolizidine building block in an efficient and eco-friendly fashion. Accordingly, we designed the stereoselective synthesis of benzo[*a*]quinolizidines using three consecutive catalytic reactions including aerobic DDQ-catalyzed allylation, Ru-catalyzed cross metathesis, and reductive cyclization. Initially, the allyl group would be installed at the α-position of nitrogen in tetrahydroisoquinoline (THIQ) via aerobic DDQ catalyzed C-C bond formation. After then, the cross metathesis reactions of the corresponding allyl compounds with vinyl ketones would provide enone, which subsequently undergoes reductive cyclization to afford benzo[*a*]quinolizidines.In this presentation, our efforts to optimize the reaction conditions and establish a series of substituted benzo[*a*]quinolizidine will be described.

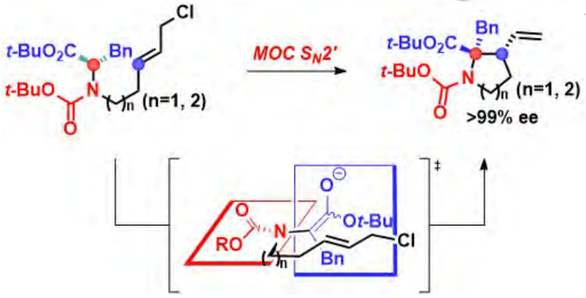
Poster Presentation : **ORGN.P-478**
Organic Chemistry
Event Hall FRI 11:00~13:00

Memory of Chirality in Intramolecular S_N2' reaction

<u>Seungbae Park</u>, Sanghee Kim[1,*]

College of Pharmacy, Seoul National University, Korea
[1]*College of Pharmacy / Department of Pharmacy, Seoul National University, Korea*

A “memory of chirality (MOC)” involved intramolecular S_N2' reaction of α-amino ester enolates with allylic halides provided a functionalized pyrrolidine and piperidine with excellent diastereo- and enantioselectivity.The MOC intramolecular S_N2' reaction provided a functionalized pyrrolidine with excellent stereoselectivity. Whereas, in the same system, the level of chirality preservation of 6-membered MOC S_N2' reactions was modest.The degree of chirality preservation of this type of intramolecular cyclization is closely related to the reaction rate. To increase the rate of MOC cyclization in piperidine system, the Thorpe–Ingold effect was employed. As a result, a high level of chirality preservation was achieved with the allylic substrate with a geminal substituent.This new method has the potential to be integrated into concise asymmetric synthesis of bioactive molecules containing multisubstituted moieties with the pyrrolidine or piperidine. Moreover, the combination of MOC cyclization and the Thorpe-Ingold effect will bring new opportunities in the area of asymmetric synthesis of cyclic compounds.



Poster Presentation : **ORGN.P-479**

Organic Chemistry

Event Hall FRI 11:00~13:00

Studies of Various Metal–Peptide Network Structures with β-Peptide or α/β-Peptide Foldamers

Seoneun Jeong, Hee-Seung Lee*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

In nature, metal-coordination is one of the important non-covalent interactions thanks to its strength and ligand selectivity. Metal-coordinated network structures fabricated from small peptidic ligands have recently received considerable attention owing to the vast structural and functional diversity of peptides. In our previous study, β-Peptide foldamers consisting of *trans*-2-aminocyclopentanecarboxylic acid (*trans*-ACPC) were used as peptide ligands with various lengths. These foldamers are decorated with 4-pyridine moieties and showed 12-helical folding propensity, even in short trimer length. The coordination of Ag^+ to the terminal pyridyl moieties afforded a set of metal-peptide networks with unique topologies. Similarly, α/β-Peptide foldamers are appropriate as peptide ligands. The Ag^+-coordination to both termini of peptide ligands formed a different network structure with wider cavities than β-peptide foldamers. α/β-Peptide foldamers composed of two types of amino acids could be substituted with different natural α-amino acid with functional groups and have a potential for applications.

Poster Presentation : **ORGN.P-480**

Organic Chemistry

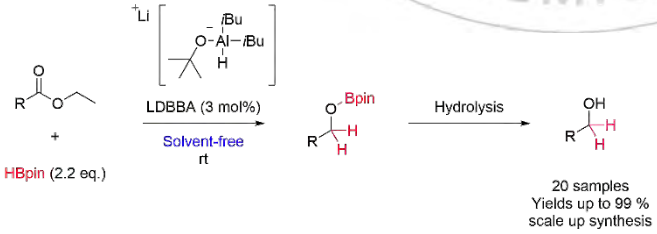
Event Hall FRI 11:00~13:00

Effective Catalytic Hydroboration of Ester with LDBBA

Hwan Hwi Kim, Hyun Tae Kim, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Hydroboration of carbonyls and unsaturated hydrocarbons have gained significant role in the synthesis of functionalized alcohols as well as other functionalities in organic synthesis. Recently, various catalytic systems were reported globally for hydroboration of carbonyls and unsaturated hydrocarbons. However, few methods were realized for relatively lower reactive functional group like esters (aldehyde > ketone > ester). Therefore, still there is need to develop methods under green protocols which includes, reactions at room temperature, less or no solvent and using readily available catalyst. Based on the above issues, our group has focused to develop simple and effective protocols for ester hydroboration. As a result, an aluminum based, lithium counter ion contained hydride reagent lithium diisobutyl- *tert*-butoxyaluminum hydride (LDBBA) was found to be efficient catalyst to promote the ester hydroboration with pinacolborane (HBpin) under solvent-free condition at room temperature. In addition, chemoselective reduction of esters was also achieved in presence of other functional groups like nitro, alkenes, and alkynes under optimized condition (Scheme).



Poster Presentation : **ORGN.P-481**

Organic Chemistry

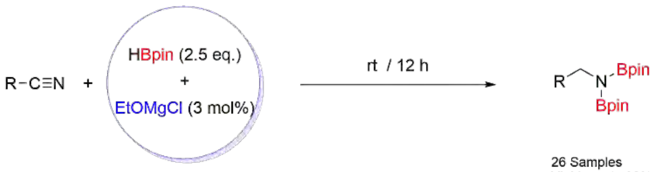
Event Hall FRI 11:00~13:00

New Catalytic Hydroboration of Nitriles using EtOMgCl as Catalyst

Ji Eun Seok, Soeun Jeon, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Hydroboration is an atom economic and straight forward reaction to obtain borylated compounds which are synthetically important intermediates in various bond forming reactions such as Buchwald, Suzuki coupling, Chan-Lam coupling, etc. In recent years much efforts were made on hydroboration of carbonyl and unsaturated (alkene and akynes) substrates with numerous catalytic systems. The reported catalytic systems are ranging from precious, transition metals to main group (*s*, *p* block) and *f*- block elements. However, relatively stable and lower reactive substrates such as nitriles require highly active metals and harsh conditions to progress the reduction due to the high dissociation bond energies associated with C≡N group. Recently, few methods on nitrile hydroboration was reported among which precious and transition metals with harsh conditions are predominant. To minimize the impact of hazardous by-products, and to reduce economic burdens, main group metals are considered as good alternatives to transition metals, available in abundantly, and possess les toxic. Herein, we wish to report hydroboration of nitriles with pinacolborane (HBpin) using readily prepared magnesium catalyst (EtOMgCl) under milder reaction conditions (low catalyst loading, room temperature) to afford N,N-diborylamines in excellent yields (Scheme).



26 Samples
Yields up to 99%

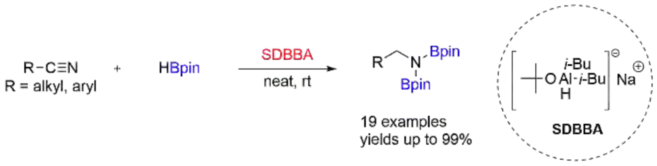
Poster Presentation : **ORGN.P-482**
Organic Chemistry
Event Hall FRI 11:00~13:00

Novel and Effective Catalytic Hydroboration of Nitriles with SDBBA Catalyst

Hwan Hwi Kim, KyungHwa Ryu, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Transformation of nitriles to value added substrates is interesting and requires more efforts as the stable and high dissociation energy of $C\equiv N$ bond (212 kcal mol^{-1}) compare to other carbonyl derivatives. Especially, synthesis of *N*,*N*-diborylamine, under catalytic reduction such as double-hydroboration is atom economic, and requires active metal catalyst to promote the reaction. Owing to the utility of resulted borylamines as synthetic precursor for C-N bond forming reactions. The hydroboration of nitrile has gained significant importance among the synthetic community and academic universities globally. As a result, hydroboration of nitriles was achieved using precious, transition metal catalyst under harsh conditions. Recently, main group metals which are economically viable and less toxic in nature were identified as an alternative to the expensive precious and transition metals for nitrile hydroboration. In continuation of our ongoing search for economically favored and sustainable reaction condition using readily available reagents, we have identified SDBBA (Sodium diisobutyl-*tert*-butoxyaluminum hydride) an aluminum based (main group and 3rd abounded in earth crust) hydride reagent has effective catalytic activity towards double hydroboration of nitrile with pinacolborane (HBpin) under room temperature (yields up to 99%). The catalyst (SDBBA) was prepared based on the reported method by our group from commercial DIBALH.



Poster Presentation : **ORGN.P-483**
Organic Chemistry
Event Hall FRI 11:00~13:00

Catalyst-free and solvent-free hydroboration of esters

<u>SuhYoun Park</u>, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Reduction of ester group to an alcohol is one of the commonly used, important reactions in small scale organic synthesis to bulk pharmaceutical industry. Generally, an ester can be reduced by using highly active aluminum reducing agents. Or metal mediated pressurized hydrogenations. In both cases, yields of the desired alcohols are often suffering in isolation process. In other words, the boron reducing agents are comparatively milder and easy to handle. Recently, hydroboration with milder reducing agent like pinacolborane (HBpin) mediated by catalytic systems are gained significant importance, owing to the less air and moister sensitive and functional group tolerance. In recent years, various catalytic systems are reported for hydroboration of esters. In continuation of our research on partial reductions and hydroboration of functional groups, we have optimized and identified an effective protocol for ester hydroboration. As a result, reaction of ester with pinacolborane has afforded corresponding boronate esters under catalyst free and solvent free condition. These boronate esters are up on hydrolysis resulted desired alcohols in good yields. Further, this method could also be smoothly applied to gram scale synthesis (Scheme).

Poster Presentation : **ORGN.P-484**

Organic Chemistry

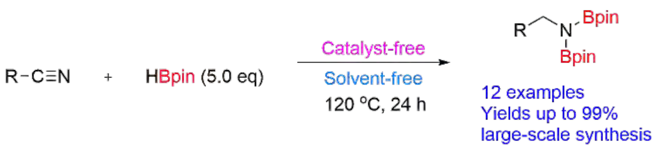
Event Hall FRI 11:00~13:00

Catalyst-free and solvent-free hydroboration of nitriles

Yongjin Lee, HyunJi Han, Duk Keun An*

Department of Chemistry, Kangwon National University, Korea

Due to the versatile industrial applications as active ingredients in various drug molecules and agrochemicals; preparation of amines from nitriles is considered as an important transformation in organic synthesis. In addition to this, reduction of nitrile with pinacolborane (HBpin) to *N*,*N*-diborylamines via double-hydroboration is atom economic and attractive reaction owing to the utility of resulted borylated amines in C-N cross coupling and amide bond forming reactions with carboxylic acid derivatives. Generally, reduction of nitriles with lower reducing agents like pinacolborane or catecholborane requires activation of reagent to promote the reaction, due to the strong dissociation energy of C≡N bond. In recent years, hydroboration of nitriles was reported with various catalytic systems such as transition, precious and main group metals. In the continuation of our research dedicated to identify economically benign, eco-friendly reaction conditions towards partial and chemoselective reductions, we have identified an effective condition for double hydroboration of nitriles under catalyst-free and solvent-free condition to obtain *N*,*N*-diborylamines in high yields. Various nitriles including gram scale hydroboration of nitriles was achieved under optimized condition (Scheme).



Poster Presentation : **ORGN.P-485**

Organic Chemistry

Event Hall FRI 11:00~13:00

Base-Mediated Allylation of *N*-2,2,2-Trifluoroethylisatin Ketimines and Its Application in Aza-Prins Reactions

<u>Ga Young Kook</u>, Haye Min Ko[*]

Department of Bio-nanochemistry, Wonkwang University, Korea

The aza-Prins reaction of allylic imines triggered by *N*-2,2,2-trifluoroethylisatin ketimine is accomplished for the synthesis of spirooxindole derivatives involving trifluoromethyl group in the presence of TMSX. This cyclization reaction is operationally simple and proceeds under mild conditions using non-toxic reagents. Notably, while the previous our work could not be compatible with TMSX (X = Cl, I, etc) in one-pot process, this work describes successful aza-Prins reaction with TMSX (X = Cl, I, etc) *via* step-by-step process.

Poster Presentation : **ORGN.P-486**

Organic Chemistry

Event Hall FRI 11:00~13:00

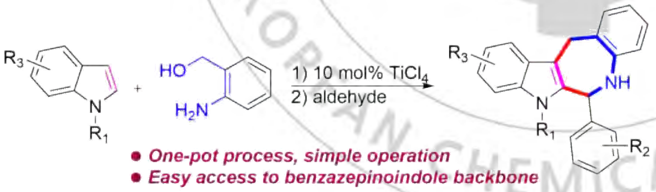
Synthesis of Benzazepinoindole Derivatives *via* a One-Pot Process of $TiCl_4$-Catalyzed Indole Alkylation/Pictet-Spengler Cyclization

Eun Ji Bang, Haye Min Ko[1,*]

Department of chemistry, Wonkwang University, Korea

[1]*Department of Chemistry, Wonkwang University, Korea*

An efficient synthetic approach involving indole alkylation/Pictet-Spengler cyclization was developed to form benzazepinoindole derivatives. The reactions proceeded smoothly with indoles, 2-aminobenzyl alcohols, and aldehydes in the presence of $TiCl_4$ as a Lewis acid catalyst. The developed one-pot protocol is operationally simple and tolerates various functional groups. Furthermore, this mild and practical tandem reaction provides a direct route to access benzazepinoindole-containing natural products and bioactive compounds.



- *One-pot process, simple operation*
- *Easy access to benzazepinoindole backbone*

Poster Presentation : **ORGN.P-487**

Organic Chemistry

Event Hall FRI 11:00~13:00

Rose bengal-sensitized cationic amphiphilic supramolecular organic photocatalyst system for efficient hydrogen evolution from seawater.

Hyun woo Nam, Soo young Park[1,*]

Materials Science and Engineering, Seoul National University, Korea

[1]*Division of Material Engineering, Seoul National University, Korea*

Photocatalytic hydrogen production through direct seawater splitting is a strategic method to lower the hydrogen production costs by skipping energy intensive desalination process. Supramolecular organic photocatalysts have attracted a lot of attention as promising materials for photocatalytic hydrogen evolution reaction (HER) because of their easy bandgap tunability, low cost, and low toxicity. Unlike reported photocatalysts (CDots/C_3N_4 nanocomposite[1] and Pt/TiO_2 granular photocatalysts[2]) that show a decrease in efficiency caused by unwanted photoredox reaction and flocculation of photocatalysts in seawater, HER efficiency of supramolecular organic photocatalysts can be enhanced by interacting favorably with many ions in seawater. Here, a panchromatic dye-sensitized supramolecular photocatalysts system was implemented by adding rose bengal (Figure 1a), an anionic dye, to improve the visible light activity of reported cation-based amphiphilic supramolecular organic photocatalysts (Figure 1b). The improved HER efficiency (~1300 µmol for 24h in simulated seawater with Pt co-catalyst and sacrificial donor ; see Figure 2) is due to the strong electrostatic interaction between the positively charged supramolecular photocatalyst and the negatively charged dye and the strong intermolecular hydrophobic interaction induced by seawater ions. This panchromatic dye sensitized supramolecular photocatalytic system may be a promising method for hydrogen production from direct seawater splitting.

Reference.

1. Liu, J.; Liu, Y.; Liu, N.; Han, Y.; Zhang, X.; Huang, H.; Lifshitz, Y.; Lee, S.-T.; Zhong, J.; Kang, Z., *Science*. 2015, *347*, 970−974.
2. Speltini, A.; Scalabrini, A.; Maraschi, F.; Sturin, M.; Pisanu, A.; Malavasi, L.; Profumo, A. *Int. J. Hydrogen Energy*. 2018, *43*, 14925–14933.

Figure 1. Molecular structures. (a) Rose bengal. (b) Cation-based amphiphilic supramolecular organic photocatalyst.

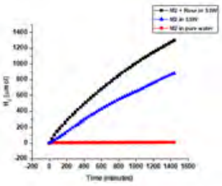


Figure 2. HER change of supramolecular organic photocatalysts according to salt and dye addition.

Poster Presentation : **ORGN.P-488**

Organic Chemistry

Event Hall FRI 11:00~13:00

Ag/Pd Bimetallic Cross Coupling Reaction of Amidoaryne Precursors and Aryl Iodides for Synthesis of Benzoxazole Derivatives

Young-Kyo Jeon, Won-SuK Kim[1,*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea
[1]*Chemistry Department of Nano-Science, Ewha Womans University, Korea*

Benzoxazoles are appealing moieties in widespread fields including pharmaceuticals and fluorescent materials. Herein, we reported Pd-catalyzed cross coupling reaction of benzoxazolylsilver intermediates for the synthesis of benzoxazole derivatives. The unprecedented key benzoxazolylsilver intermediate is formed by silver fluoride mediated intramolecular oxyargentation of amidoaryne precursors. Subsequent Pd-catalyzed coupling reactions of aryl iodides with an in situ generated silver intermediate allowed facile access to valuable C7-arylated benzoxazole derivatives with broad functional group tolerance and substrate scope. Mechanistic studies have shown that controlling the timing between benzyne formation/oxy-argentation and transmetalation is a significant factor in the reaction system. Notably, it was found that the position of silyl group is important for benzyne formation because C-Si bond cleavage by AgF is affected by possibility of 1,5-Brook rearrangement and C-Si bond strength depending on the position of the silyl group.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-489**
Organic Chemistry
Event Hall FRI 11:00~13:00

Site-Selective C–H Pyridylation of Unactivated Alkanes via Photocatalysis

<u>Wooseok Lee</u>, Sungwoo Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Site-selective functionalization of C–H bonds using visible light is a challenging reaction in the field of chemical research. In this research, we design a new synthetic route for the site-selective C–H pyridylation of unactivated hydrocarbons by using direct hydrogen atom transfer catalyst with reverse hydrogen atom transfer reagent. The selective pyridylation of more substituted, electron-rich C–H bonds in abundant chemical feedstocks was achieved by pyridinium salts. We provide a new catalytic system for the direct construction of valuable compounds under ambient reaction conditions. Moreover, this method enables functionalization in a wide range of fields from general alkane feedstocks under mild, metal-free reaction conditions.

Poster Presentation : **ORGN.P-490**

Organic Chemistry

Event Hall FRI 11:00~13:00

Visible-light-Induced Conversion of Alkenes to Branched or Linear Alkyl pyridines

Minseok Kim, Sungwoo Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

We report a pragmatic protocol for the visible-light-induced radical-mediated regiodivergent hydropyridylation of unactivated alkenes using N-aminopyridinium salts. It is noteworthy that this approach provides a unified synthetic platform to control the regioselectivity of the synthesis of linear or branched C4-alkylated pyridines. A remarkable selectivity switch from the anti-Markovnikov to the Markovnikov product can be accomplished by the addition of tetrabutylammonium bromide. The versatility of this strategy is further demonstrated based on the late-stage functionalization in complex molecules such as pharmaceuticals.

Poster Presentation : **ORGN.P-491**

Organic Chemistry

Event Hall FRI 11:00~13:00

Studies on synthesis of N-acyl amidines and reactivity of the [3 + 2] cycloaddition according to functional groups

Shinjae Lee, Seewon Joung[1,*]

Department of chemistry, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

The cyclic amidines structures have been observed in natural products and various biological inhibitors. Based on these potential biological activities of the cyclic amidines, we tried to synthesize various cyclic amidines using acyl azide and sulfonyl azide. In our previous study, borane catalyst and silane were used to create an N-silyl enamine intermediate through hydrosilylation. By adding sulfonyl azide to the reaction mixture, we could induce [3 + 2] dipolar cycloaddition reaction to form the cyclic amidines. However, acyl azide was relatively less reactive than sulfonyl azide, so the yield of cyclic amidines using acyl azide was poor. Therefore, we decided to increase the reactivity of the acyl azide by attaching electron withdrawing substituent to the acyl azide. Also we studied the reactivity of the N-silyl enamines and acyl azides with various electronic nature.

Poster Presentation : **ORGN.P-492**

Organic Chemistry

Event Hall FRI 11:00~13:00

A Nucleophilic Iridium–Nitrenoid

Bohyun Park, Mu-Hyun Baik*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Group IX metal–nitrenoid such as Rh=NC(O)R or Ir=NC(O)R is a key intermediate during the C–H amidation using dioxazolone family. According to tons of studies by Chang and other groups, it is well known that the metal–nitrenoid has an electrophilic nature so that it could easily undergo reductive C(sp^3)–N or C(sp^2)–N coupling. Unlike conventional alkyl or aryl amidations, in our previous study with the Blakey group, we doubted that the metal–nitrenoid might attack the allylic carbon in a nucleophilic fashion. Herein, we suggest that the iridium–nitrenoid is not only electrophilic but could be also nucleophilic depending on the coupling partner. The demonstration of the nucleophilic character of the iridium–nitrenoid will be shown with some proof from both computational and experimental studies.

Poster Presentation : **ORGN.P-493**

Organic Chemistry

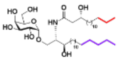
Event Hall FRI 11:00~13:00

Synthesis of host immunomodulatory lipids created by symbionts

Yoon Soo Hwang, Jesang Lee, Sungwhan F. Oh[1,*], Seung Bum Park[*], Dennis L. Kasper[2,*]

Department of Chemistry, Seoul National University, Korea
[1]*Department of Anesthesiology, Brigham and Women′s Hospital, U.S.A., United States*
[2]*Department of Immunology, Blavatnik Institute of Harvard Medical School, U.S.A., United States*

Small molecules derived from symbiotic microbiota critically contribute to intestinal immune maturation and regulation. However, little is known about the molecular mechanisms that control immune development in the host–microbiota environment. Here, we carried out an organic synthesis to support a multifaceted investigation of immunomodulatory α-galactosylceramides from the human symbiont Bacteroides fragilis (BfaGCs). Considering the structural diversity of gut commensal sphingolipids, we designed and prepared 23 BfaGC isomers with different chain lengths (C15–C19) and terminal branching (iso- or anteiso-). During a total synthesis, optimized synthetic route of BfaGCs was developed and will be utilized in further studies.With BfaGC analogue library, our coworkers revealed that the sphinganine chain branching of BfaGCs was a critical determinant of natural killer T (NKT) cell activation and SB2217 which contains branched sphinganine showed unique immunomodulatory functions. Consequentially, this study presented a structural and molecular-level paradigm of immunomodulatory control by interactions of endobiotic metabolites with diet, microbiota and the immune system.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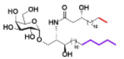
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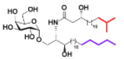
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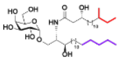
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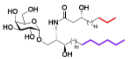
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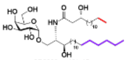
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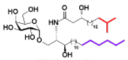
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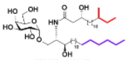
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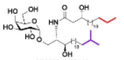
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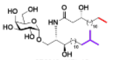
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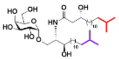
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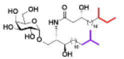
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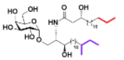
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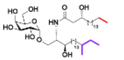
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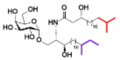
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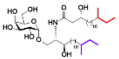
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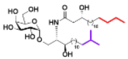
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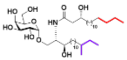
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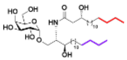
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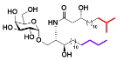
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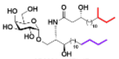
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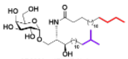
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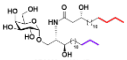
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Poster Presentation : **ORGN.P-494**

Organic Chemistry

Event Hall FRI 11:00~13:00

Antiaromatic Macrocycle-based Metal Organic Framework

<u>Minkyu Song</u>, Woo-Dong Jang[*]

Department of Chemistry, Yonsei University, Korea

Antiaromaticity can plays key role in narrowing the bandgap of organic materials. A planar β,β'-phenylene-bridged *Meso*-aryl hexaphyrins (1.0.1.0.1.0), a 24 π-electron antiaromatic expanded porphyrinoids (**Py$_3$Ros**) was synthesized. Through a redox reaction, **Py$_3$Ros** can change its aromaticity. Therefore, the absorption can be changed during the redox process. By using antiaromatic **Py$_3$Ros** as an organic building block, Metal-Organic Frameworks (MOFs) was synthesized. Through the interfacial synthesis method, MOFs having microcrystalline structure was successfully obtained. Synthesized MOFs also showed changes in the absorption spectrum through the redox reaction. We expect these **Py$_3$Ros**-based MOFs can be applied in the electronic devices.

Poster Presentation : **ORGN.P-495**

Organic Chemistry

Event Hall FRI 11:00~13:00

Porphyrin-based Covalent Organic Framework for photochemical CO2 reduction

<u>Hansung Ko</u>, Jehee Lee, Tae Kyu Kim*, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Covalent organic framework (**COF**) is a material based on covalent bonding of organic precursors. COF has high porosity and crystallinity, is conductively studied in various application fields. Porphyrins are useful precursors for fabrication of functional COF and central metal can be easily introduced to the porphyrin structure during the synthetic procedure. A porphyhrin-based COF (**PCOF**) was synthesized through the imine condensation reaction of tetraaminophenyl porphyrin (**T$_A$PP**) and diformylphenyl porphyrin (**D$_F$PP**). Thus obtained COF was characterized by PXRD and TEM analysis. A photocatalytic CO_2 reduction reaction was conducted using **PCOF**. The CO_2 reduction reaction using **PCOF** showed high CO yield and good CO/H_2 selectivity. Based on this result, it can be expected to show better CO conversion efficiency and selectivity, when combining **T$_A$PP$_{Cu}$** and **D$_F$PP** with various metals.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-496**

Organic Chemistry

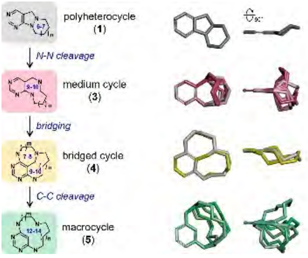
Event Hall FRI 11:00~13:00

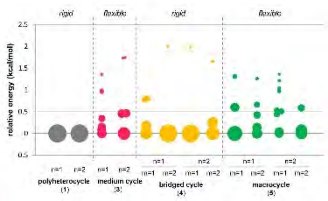
Design and synthesis of conformationally diverse pyrimidine-embedded medium/macro- and bridged cycles *via* skeletal transformation

Subin Lee, **Seung Bum Park***

Department of Chemistry, Seoul National University, Korea

The rigidity and flexibility of small molecules can be critical for 3-dimensional ligand-protein interaction. The orientation of essential substituents can be pre-organized in the conformationally rigid small molecules, so they might interact with specific biological targets selectively. On the other hand, the conformationally flexible small molecules enable distinct binding modes for different proteins due to equilibrium between different conformations. Therefore, small-molecule libraries with conformational diversity would be an invaluable resource for studying the influence of skeletal flexibility on the biological system. Here, we designed and synthesized ten skeletally and conformationally diverse medium/macro- and bridged cyclic scaffolds containing 7 to 14-membered rings via an efficient skeletal transformation strategy. Furthermore, we conducted some chemoinformatic analysis to confirm their high shape and conformational diversity compared to the known pyrimidine-embedded bioactive compounds.





Poster Presentation : **ORGN.P-497**

Organic Chemistry

Event Hall FRI 11:00~13:00

Development of Green to Red-emitting BODIPY-Tetrazine Fluorogenic Probes with a Monochromophoric Design Strategy

Hayoung Son, Dahham Kim[1], Seung Bum Park[1,*]

Department of Chemistry, Seoul National University, Korea

[1]*Division of Chemistry, Seoul National University, Korea*

For fluorescent bioimaging, fluorogenic bioprobes are beneficial owing to their low background signals and handy wash-free property. By taking advantage of tetrazine (Tz) as a fluorescence quenching unit and a bioorthogonal reaction moiety, a fluorophore−Tz conjugate (FLTz) has been utilized for fluorescent live cell imaging via inverse electron-demand Diels−Alder (iEDDA) bioorthogonal reaction. Nevertheless, most FLTz fluorogenic probes rely on wavelength dependent bichromophoric energy transfer quenching mechanisms, which constrain red-shifting of probes' emission wavelength without deterioration of the fluorescent turn-on/off ratio. To address this limitation, herein we develop a series of new Green to Red-emitting BODIPY-Tz derivatives designed with a monochromophoric design strategy to bear an excellent fluorogenic property. The designed BODIPY-Tz probes are successfully utilized as an imaging tool in mammalian cells.

Poster Presentation : **ORGN.P-498**

Organic Chemistry

Event Hall FRI 11:00~13:00

Transition-Metal-Free Funtionalization of Benzoxazinones using 1,4-Dihydropyridines

Junghyea Moon, In Su Kim*

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

The direct functionalization of N-heterocycles is a vital transformation for the development of pharmaceuticals, functional materials, and other chemical entities. Herein, the transition-metal-free alkylation and acylation of C(sp2)–H bonds in biologically relevant 2-benzoxazinones with 1,4-dihydropyridines as readily accessible radical surrogates is described. Excellent functional group compatibility and a broad substrate scope were attained. Gram-scale reaction and transformations of the synthesized adducts via Suzuki coupling with heteroaryl boronic acids demonstrated the synthetic potential of the developed protocol.

Poster Presentation : **ORGN.P-499**

Organic Chemistry

Event Hall FRI 11:00~13:00

Mechanically-Coupled Rotary Motions of Molecular π-Stacks

Hongsik Kim, Dodam Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Dynamic non-covalent assembly has been a long-standing interest in chemistry. One of the most frequently found structure-organizing principles in these supramolecular systems is intimate contact between aromatic rings. In synthetic chemistry, however, the coexistence of fluxionality and thermodynamic stability of π-stacks still remains challenging because of the dispersive and distance sensitive nature of π–π interactions. As an intuitive solution to build fluxional π-stacks, we designed conformationally well-defined molecular triple-deckers featuring aryl–naphthyl–triazolyl motif. The judiciously designed spacing between juxtaposed aromatic fragments enabled dynamic shuffling of π-stacks while maintaining their vertical alignment as well. A combination of X-ray crystallographic, 1D/2D/VT NMR spectroscopic, and density functional theory (DFT) computational studies revealed that mechanically-coupled rotary motion is the underlying mechanism of the fluxionality. By VT fluorescence and time-resolved photoluminescence measurements, we further demonstrated the critical functional role of floor-changing motions to control the excited-state structural dynamics and its photophysical consequences.

Poster Presentation : **ORGN.P-500**
Organic Chemistry
Event Hall FRI 11:00~13:00

Sequence-Specific Supramolecular Self-Assembly: Rational Design of π-Clips to Build Columnar π-Stacks

Hyun Lee, Dongwhan Lee[1,*]

Chemistry, Seoul National University, Korea
[1]*Division of Chemistry, Seoul National University, Korea*

With electronic coupling between molecular building blocks, columnar π-stacks of aromatics can be engineered into electronic and optical materials. To build stacked multi-layer aromatics with well-defined orientation and vertical sequence, we have designed and synthesized a series of C-shaped molecules with spatially preorganized π-surfaces. With shape complementarity, the two parallel-oriented π-surfaces and hydrogen bonds synergistically reinforce each other to afford a–b–b–a type π-sequence stacks by self-dimerization in the solution phase. Comparative studies of a homologous set of molecules having structurally varied upper canopies demonstrated that subtle changes in the non-covalent interactions determine the dimerization propensity. This shape-dependent property was investigated by a combination of X-ray crystallographic, NMR spectroscopic, and computational studies. To build an “infinite” π-stack by non-covalent polymerization, we further synthesized an S-shaped molecule having two non-collapsible pockets. This presentation will discuss key design principles to exploit conformational pre-organization and synergistic non-covalent interactions to control the long-range structural arrangement of molecular π-stacks.

Poster Presentation : **ORGN.P-501**

Organic Chemistry

Event Hall FRI 11:00~13:00

Systematic exploration of furoindolizine-based molecular framework towards a versatile fluorescent platform

Youngjun Lee, Dahham Kim[1], Seung Bum Park[1,*]

Department of Chemistry and Biochemistry, University of California, San Diego, United States

[1]*Division of Chemistry, Seoul National University, Korea*

The photophysical behaviors of fluorescent molecules largely determine their major utility in biological studies. Classical fluorophores have been utilized with good brightness and general applicability, but sometimes challenged with limited synthetic methodology and tunability to adjust intrinsic optical properties despite their well-defined characteristics. A new heterocyclic core equipped with modular functional groups may offer a flexibility to control its photophysical properties with a minimum synthetic effort. By conducting a systematic analysis guided by quantum calculations, we proposed the furoindolizine-based molecular framework as a unique fluorescent platform for versatile photophysical properties with minimal structural modification. Furoindolizine derivatives exhibited broadly tunable photophysical properties such as emission wavelength, stokes shift, fluorescent brightness, and charge transfer characteristics using synergistic interaction between two functional moieties. Furthermore, this modular platform enabled secure live-cell imaging probes with two distinct optical features simply by reorganizing a pair of functional moieties.

Poster Presentation : **ORGN.P-502**

Organic Chemistry

Event Hall FRI 11:00~13:00

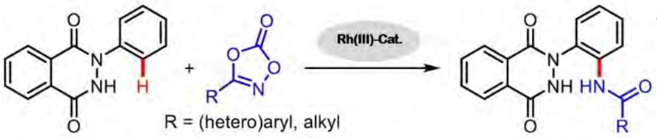
Rh(III)-Catalyzed C-H Amidation of Phthalazinone using Dioxazolones

<u>Suho Kim</u>, In Su Kim[1,*]

Sungkyunkwan University, Korea

[1]*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

There are so many heterocycles in nature, containing nitrogen and closely related to heterocyclic medicinal applications. The phthalazinone skeleton is ubiquitous structural motif, which plays a central role in pharmaceutics; anti-inflammatory, anti-microbial, etc. Till now, the catalytic C−H amination has been used in the most ways for synthesis of the N-heterocyclic compounds. And currently, the new schematic method with phthalazinone derivatives via transition-metal catalysis has been developed. Although the new methods with phthalazinone derivatives via transition-metal catalysis developed, they have been used on the C−C bond formation with π-unsaturated substrates and N-aryl phthalazinones limitedly. By using a transition-metal catalysis; rhodium(III) and an amide source; dioxazolones, we propose the new method the C−N bond formation of N-aryl phthalazinones in the catalytic C−H amination. The new method can be used in various way, especially the bioactive compound in drug discovery.



Poster Presentation : **ORGN.P-503**

Organic Chemistry

Event Hall FRI 11:00~13:00

Dicationic Amphiphiles for Anion-Induced and Aggregation-Enhanced Light Emission: Tailoring Hydrophobicity to Distinguish Non-Coordinating Anions

Chungryeol Kim, Soohyung Kim, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Chemistry of non-coordinating anions have been widely utilized in catalysis, ionic liquids, and energy storage. Nevertheless, general principles to distinguish such anions still remain elusive. In particular, molecular level recognition of hydrophobic anions beyond the classical Hofmeister series in water is challenging because water molecule itself effectively attenuates electrostatic or ion-dipole interactions. We now disclose an optical method to distinguish hydrophobic anions in water by using dicationic fluorophores. Ion pairing with large and charge-diffuse anions results in salt aggregation, which elicits a dramatic fluorescence enhancement. Depending on the chemical structure of the anions, different response profiles were observed. Furthermore, we demonstrate that both the sensitivity and selectivity of the fluorophore toward various anions can be controlled by systematically changing the hydrophobicity by varying the length of peripheral alkyl chains. In this presentation will be discussed key design principles, synthetic implementations, and practical applications of designer molecules for the detection of hydrophobic anions in water.

Poster Presentation : **ORGN.P-504**

Organic Chemistry

Event Hall FRI 11:00~13:00

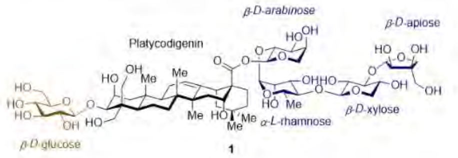
Synthesis and Structure-Activity Relationship of Saponin-Based Membrane Fusion Inhibitors against SARS-CoV-2

Young Ho Jang, **Sunkyu Han***

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

An ongoing pandemic of coronavirus disease 2019 (COVID-19) is now the greatest threat to global public health. Herbal medicines and their derived natural products have drawn much attention in the treatment of COVID-19, but the detailed mechanisms by which natural products inhibit SARS-CoV-2 have not been elucidated. Here, we show that platycodin D(PD) effectively blocks the two main SARS-CoV-2 infection routes via lysosome- andtransmembrane protease serine 2 (TMPRSS2)-driven entry. Mechanistically, PD prevents host entry of SARS-CoV-2 by redistributing membrane cholesterol to prevent membrane fusion, which can be reinstated by treatment with a PD encapsulating agent. In this study, we synthetically assess the potential of saponin derivatives (natural and synthetic) as inhibitor against SARS-CoV-2 and the synthetic saponin inhibitory activity is roughly 3-fold higher than platycodin D.

Structure of Platycodin D and Key structural components



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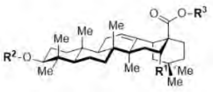
Semisynthesis saponin derivatives



	R^1	R^2	R^3
2	H	β-Glc	H
3	H	β-Glc	β-Ara
4	H	β-Glc	β-Xyl-(1′|3)-β-Xyl
5	H	β-Glc	β-Xyl-(1′|3)-β-Xyl-(1′|3)-β-Xyl-(1′|3)-β-Xyl
6	H	β-Glc	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
7	H	OH	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
8	OAc	β-Glc	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
9	OAc	OH	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
10	OH	β-Glc	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
11	OH	Bn	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
12	OH	β-Glc	β-Xyl-(1′|3)-β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara
13	OH	β-Glc	β-Xyl-(1′|3)-β-Xyl-(1′|4)-α-Rha-(1′|2)-β-Ara-OCH_2

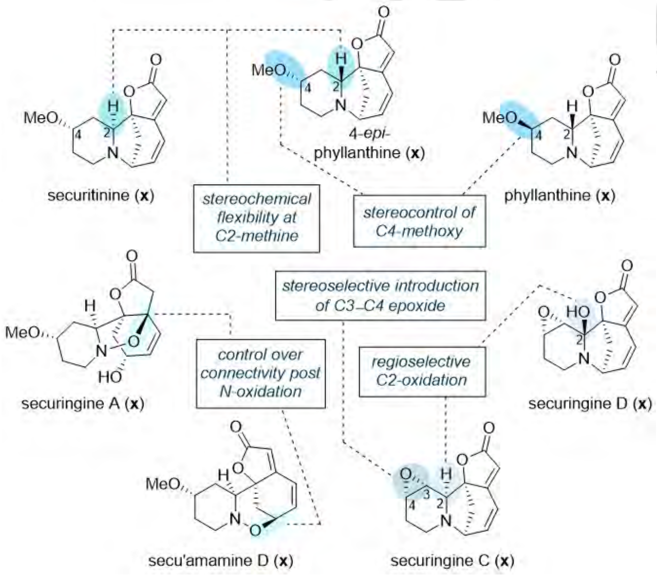
Poster Presentation : **ORGN.P-505**
Organic Chemistry
Event Hall FRI 11:00~13:00

Collective Total Synthesis of High-Oxidation State Securinine-Type Alkaloids

Sangbin Park, Sunkyu Han*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

High-oxidation state securinega alkaloids are additionally oxidized metabolites from the fundamental core of securinega natural products. This system shows complex oxidation patterns according to various oxidation at different sites of the securinega structure. Among this securinega alkaloids, the members containing prperidine-based ring are called securinine-type alkaloids. Securinine-type alkaloids can undergo biosynthetic oxidations to yield various high-oxidation state securinine-type with oxidative decorations around the piperidine scaffold (N1, C2–C4). Inspired by these biosynthetic oxidations, we strategized divergent synthesis of high-oxidation state securinine-type alkaloids via various oxidations, rearrangement, and epimerization around the piperidine core of securinine scaffolds. Among them, the total synthesis of securitinine, securingines A, C, D, secu’amamine D, 4-epi-phyllanthine, and phyllanthine has been achieved. Our research provides a general synthetic solution to all known securinine-type alkaloids.



Poster Presentation : **ORGN.P-506**

Organic Chemistry

Event Hall FRI 11:00~13:00

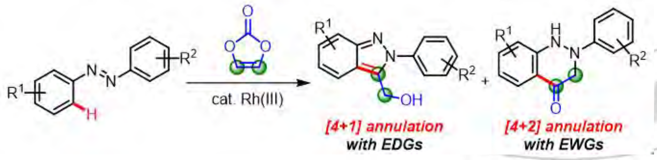
Synthesizing (2H)-Indazoles and Dihydrocinnolinones via Rh(III) Catalyzed Annulation of Azobenzenes with Vinylene Carbonate

Kyeongwon Moon, In Su Kim[1,*]

School of Pharmacy, Sungkyunkwan University, Korea

[1]*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

The Rh(III)-catalyzed C–H functionalization and subsequent intramolecular cyclization between azobenzenes and vinylene carbonate is described herein. Depending on the electronic property of azobenzenes, this transformation results in the formation of (2H)-indazoles or dihydrocinnolin-4-ones through the generation of ortho-alkylated azo-intermediates followed by decarboxylation. Surprisingly, vinylene carbonate acts as an acetaldehyde or acetyl surrogate to enable the [4+1] or [4+2] annulation reaction. This transformation is characterized by its mild reaction conditions, simplicity, and excellent functional group compatibility.



Poster Presentation : **ORGN.P-507**

Organic Chemistry

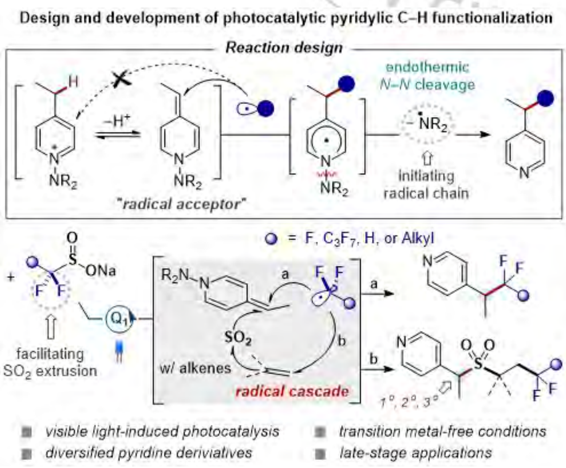
Event Hall FRI 11:00~13:00

Visible Light-Induced Pyridylic C–H Functionalization via Radical Cascades

Myojeong Kim, Sungwoo Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Under visible light photocatalytic conditions, an efficient pyridylic C(sp^3)–H functionalization has been achieved through radical fluoroalkylation or radical-mediated cascade reactions. This approach is enabled by the reversible formation of alkylidene dihydropyridine intermediates via the enolate formation of C4-alkyl *N*-amidopyridinium salts in the absence of an external base, thereby establishing the conditions essential for subsequent intermolecular radical trapping. Rapid structural diversification of the pyridylic site was enabled by cascade reactions involving alkene trifluoromethylation, SO_2-reincorporation, and the addition of the produced sulfonyl radical. This operationally simple protocol is applicable to a broad substrate scope and high chemoselectivity, and offers a unique approach for the rational modification of the heterobenzylic C–H bonds of pyridines and quinolines in a highly selective fashion. Furthermore, experimental studies and theoretical calculations were performed to elucidate the reaction mechanism.



Poster Presentation : **ORGN.P-508**

Organic Chemistry

Event Hall FRI 11:00~13:00

A Novel Supramolecular Eutectic Liquid as Precursor for Several Type of Carbon Materials Synthesis

Dhita Azzahra Pancorowati, Chiyoung Park[1,*]

Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Carbon materials (CMs) exhibit great application potential in diverse fields owing to their remarkable properties, like: high electrical conductivity, good chemical stability, and unique microstructure. In this work, we introduce a novel supramolecular eutectic liquid (EL) as precursor for CMs with simple and low-cost synthesis process which can produce various type of CMs. We present three different type of synthesis route: 1) By simple carbonization process of EL, we were able to produce shiny-surface glassy carbon film with high electrical conductivity of 4510 S/cm. 2) By add metal as the catalyst in carbonization process, we were success to produce multi-layer graphene with the absence of defect band on its structure. 3) We have utilized flame soot synthesis process to produce carbon black with particle size range from 50 – 70 nm. In addition, this carbon can be used as oxidation resistant coating on metal such as copper wire.

Poster Presentation : **ORGN.P-509**

Organic Chemistry

Event Hall FRI 11:00~13:00

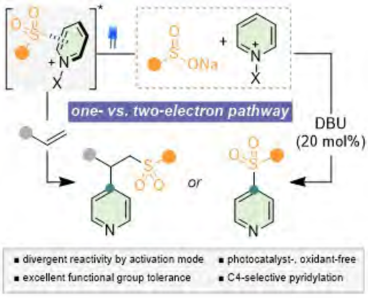
Divergent Synthetic Strategy of Sulfinates and Pyridinium Salts on the Basis of one- *versus* two-electron pathways

Euna You, Sungwoo Hong[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

One of the main purposes for modern organic chemistry is that develop distinct reaction pathways from the same starting materials to synthesize diverse compounds. We report the divergent synthetic application of sulfinates with pyridinium salts to achieve the sulfonative pyridylation of alkenes and direct C4-sulfonylation of pyridines by controlling the one- *versus* two-electron pathways for selective formation of each product. Base-catalyzed coupling reaction between sulfinate and *N*-amidopyridinium salt can be directly incorporated sulfonyl group to C4 position of pyridine. Importantly, The reactivity of this set of compounds is completely converted upon irradiation to visible light: electron donor-acceptor (EDA) complexes of *N*-amidopyridinium salts and sulfinates can access to sulfonyl radical. In this catalyst-free radical pathway, both sulfonyl and pyridyl group could be inserted into alkenes through a three-component reaction, which offer facile access to various β-pyridyl alkyl sulfones. These two reactions are orthogonal and complementary, exhibiting a wide range of substrate scopes and late-stage modification under mild conditions.



Poster Presentation : **ORGN.P-510**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Small-Molecule Fluorescent Probes for Imaging of OGA

Chaeyeong Lee, **Ghilsoo Nam**[1,*]

Depart of Chemistry, Korea University, Korea
[1]*Korea Institute of Science and Technology, Korea*

O-GlcNAcylation, which is a dynamic glycosidic addition of O-linked N-acetylglucosamine(O-GlcNAc) to nucleocytoplasmic proteins, is one of the post-translation modifications(PTMs) distributed in cytosol, nucleus and mitochondria. Unlike phosphorylation, this reversible modification is principally governed by two enzymes; O-GlcNAc transferase(OGT), which couples O-GlcNAc to the acceptor protein; and O-GlcNAcase(OGA) that hydrolyses this action. A Disproportion of O-GlcNAc levels is physiologically associated with numerous chronic diseases in human such as cancer, diabetes and neurodegeneration. While an interest in O-GlcNAcylation for medicinal purposes is increasing, compared to OGT Activity assay, only few fluorophores were reported to monitor OGA relatively. In present work, we synthesized small-molecule fluorescent probes(RSF-Glu, AMC-Glu) for monitoring of OGA activity. We expected that probes could serve as a direct and effective sensor for OGA activity.

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April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-511**

Organic Chemistry

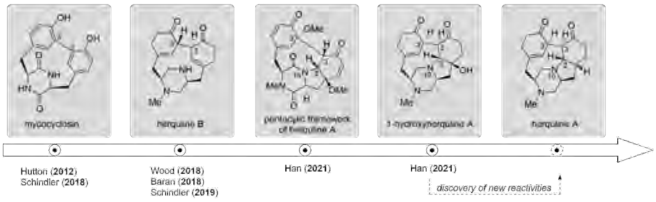
Event Hall FRI 11:00~13:00

Synthesis and Reactivities of 1-Hydroxyherquline A

<u>Chungwoo Lee</u>, Sunkyu Han*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The highly strained bowl-shaped pentacyclic structure of herquline A has rendered it one of the most difficult problems in organic synthesis yet to be solved. The challenges associated with the synthesis of herquline A have been well documented in four Ph.D. dissertations and in multiple reports regarding syntheses of its structurally simpler congeners. Herein, we report the construction of the pentacyclic core of herquline A, the synthesis of 1-hydroxyherquline A and describe its reactivities discovered en route to its attempted conversion to herquline A.First, we were able to synthetically access the pentacyclic framework of herquline A that contains both N10-C2 and C3-C3’ bonds. The key for success was the development of the tandem aza-Michael addition/enolate capture protocol that set the stage for subsequent palladium catalyzed C3(sp^2)-C3’(sp^2) coupling reaction. Ensuing oxidative dearomatization of the left aryl ring allowed the formation of the pentacyclic diketone core of herquline A. By revising the synthetic approach, we could next synthesized 1-hydroxyherquline A, the most advanced herquline A congener reported to date. Strategic installation of the C1-hydroxyl group enabled the key *aza*-Michael addition mediated N10-C2 bond formation. Our attempted reductive transformation of 1-hydroxyherquline A to herquline A was challenged by the exteremly strained bowl-shaped pentacyclic structures of key precursors that prevented either the radical formation at C1 or the protonation/hydrogenation from the desired face. We believe that these discoveries would serve as guiding lights toward this formidable target.



Poster Presentation : **ORGN.P-512**

Organic Chemistry

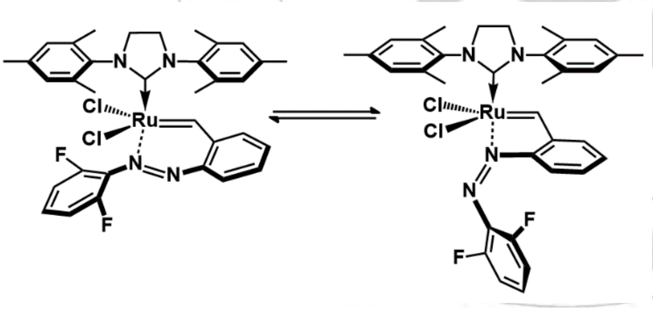
Event Hall FRI 11:00~13:00

Study of the photo-controllable catalytic activity of azobenzene containing Ru olefin metathesis catalyst

Dayong Song, Cheoljae Kim[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk National University, Korea*

We have synthesized a Ru olefin metathesis catalyst bearing fluorine-substituted azobenzene on benzylidene part to coordinate the Ru metal. The synthesized Ru catalyst complex showed photoisomerization in the presence of blue LED, and the structure was determined by ^{1}H NMR. The research is ongoing to use this catalyst complex for the photo-triggered reaction.



Poster Presentation : **ORGN.P-513**

Organic Chemistry

Event Hall FRI 11:00~13:00

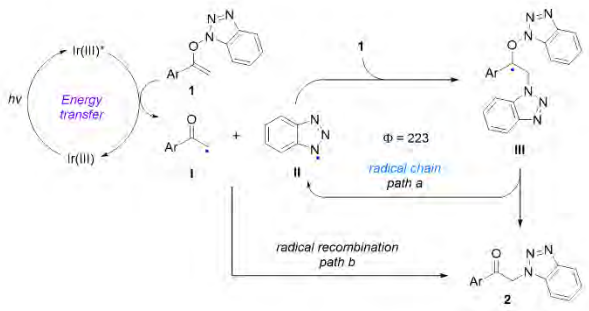
1,3-O to C-Benzotriazole Shift of N-enoxybenzotriazoles: Generation of N-centered Radical via Energy Transfer

Huong Quynh Nguyen, **Seunghoon Shin**[1,*]

Chemistry, Hanyang University, Korea

[1]*Department of Chemistry, Hanyang University, Korea*

Nitrogen-centered radicals are a versatile class of reactive species that can undergo various radical transformations.[1] In recent decades, photolytic catalysis has emerged as a powerful method to render a diverse range of radical intermediates. Toward this end, we introduced a photocatalysis reaction employing N-enoxybenzotriazoles. Upon visible-light irradiation, the triplet-triplet energy transfer could trigger N-O bond homolytic fragmentation of the N-enoxybenzotriazoles affording an α-carbonyl radical and a benzoytriazolyl radical. The resulting benzotriazolyl radicals underwent a formal 1,3-O to C-shift generating a variety of α-benzotriazolyl ketones.[3] Despite the comprehensive development of nitrogen-centered radicals, generation and synthetic utility of benzotriazolyl radicals has been underexplored. Benzotriazoles and their derivatives possess a broad range of pharmacological reactivity.[2] Thus, the benzotriazole-incorporated products could be of potential benefits for the relevant drug discovery.References1. (a) Xiong, T.; Zhang, Q. *Chem. Soc. Rev.* **2016**, *45*, 30692; (b) Jiang, H.; Studer, A. *CCS Chem.* **2019**, 38; (c) Yu, X. Y.; Zhao, Q. Q. *Acc. Chem. Res.* **2020**, *53*, 1066. 2. (a) Suma, B.; Natesh, N.; Madhavan, V. J. *Chem. Pharm. Res.* **2011**, *3*, 375; (b) Briguglio, I.; Piras, S.; Corona, P.; Gavini, E.; Nieddu, M.; Boatto, G.; Carta, A. *Eur. J. Med. Chem.* **2015**, *97*, 612.3. Q. H. Nguyen; Shin, S. *manuscript in preparation.*


hν
Ir(III)*
Energy transfer
Ir(III)
Ar
1
I
+
II
Φ = 223
radical chain
path a
III
radical recombination
path b
2

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-514**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of pyrazoline derivatives from N-silyl enamine and nitrile imine

Sooyeon Yun, Seewon Joung[1,*]

Department of chemistry, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

Enamines can be utilized for the synthesis of amines, amidines, and other nitrogen containing functional groups, showing a variety of applicability for organic synthesis and medicinal chemistry. Our previous studies have focused on the synthesis of cyclic amidines using organic azides with enamine intermediates from the borane catalyzed hydrosilylation of isoquinolines and quinolines. This study is about construction of pyrazoline ring by using [3 + 2] cycloaddition of the nitrile imine with the N-silyl enamine from the readily available N-heteroarenes.

Poster Presentation : **ORGN.P-515**

Organic Chemistry

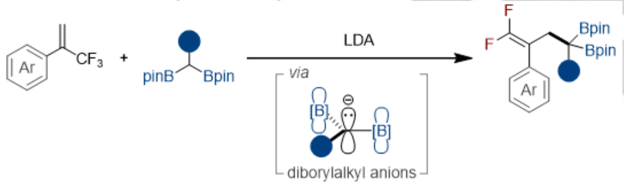
Event Hall FRI 11:00~13:00

Transition-Metal-Free Defluorinative C−C Bond Forming Reaction of Trifluoromethyl Alkenes with *gem*-(Diborylalkyl)lithium Species

Haeun Kim, Seung Hwan Cho[*]

Department of Chemistry, Pohang University of Science and Technology, Korea

We report the transition-metal-free defluorinative C−C bond forming reaction of trifluoromethyl alkenes with *gem*-(diborylalkyl)lithiums. This synthetic strategy gives access to various 4,4-difluoro homoallylic diboronate esters, which serve as versatile intermediates for the preparation of valuable *gem*-difluoroalkene derivatives in good efficiency. Further synthetic modifications are conducted to showcase the synthetic usefulness of the obtained 4,4-difluoro homoallylic diboronate esters.



Poster Presentation : **ORGN.P-516**

Organic Chemistry

Event Hall FRI 11:00~13:00

pH-Dependent Anion Recognition in Water: Systematic Approaches to Understand and Exploit Aggregation-Induced Fluorescence Enhancement

Soohyung Kim, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Molecular recognition in water is an unperfected art in synthetic supramolecular chemistry. In particular, the recognition of anions in water remains a key challenge. With appropriate molecular design, anion-responsive fluorophores allow for selective and sensitive detection. They can also be switched on and off under specific conditions such as changes in pH. We have devised multipodal polycationic molecules functioning as anion-responsive light-emitters. In water, ion–pairing and aggregation event elicited a selective fluorescence "turn on" response toward hydrophobic anions. By systematically varying the alkyl pendants, we demonstrated that the response profile and threshold of the signaling event could be modulated at the molecular level. Moreover, by installing pH-responsive functional groups at the alkyl chains, the fluorescence signaling events are controlled at specific pH. In this presentation will be discussed key design principles, synthetic implementations, and rational strategies to realize pH-responsive detection of specific anions in water.

Poster Presentation : **ORGN.P-517**

Organic Chemistry

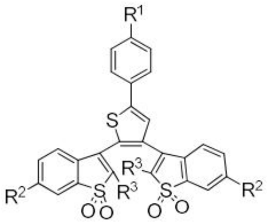
Event Hall FRI 11:00~13:00

Photochromic properties of diarylethene with electron donor/acceptor substituents

Tae Ho Youn, Kwang-Hyun Ahn[1,*]

Applied chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Diarylethene compounds are well known for its photochromic properties. Various studies have been conducted on compounds with these characteristics.In this study, we are trying to focus on the characteristics of diarylethenes with electron donor/acceptor substituents. We will discuss about various physical properties of diarylethenes including fluorescence switching efficiency. The substituent effect on the photochromic properties will also be presented.



129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-518**

Organic Chemistry

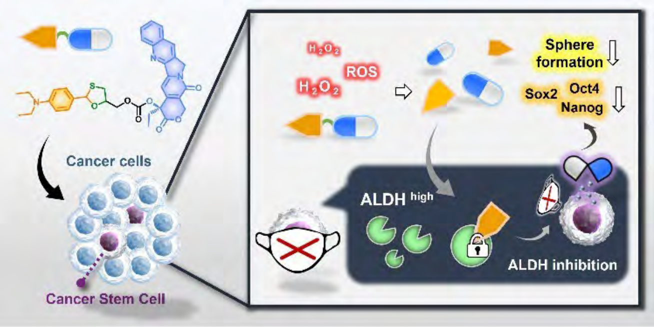
Event Hall FRI 11:00~13:00

ROS activable prodrug for aldehyde dehydrogenase overexpressed cancer stem cells

Miae Won, Ji Hyeon Kim[1], Jongseung Kim[1,*]

R&D institute, TheranoChem Inc., Korea
[1]Department of Chemistry, Korea University, Korea

Aldehyde dehydrogenase (ALDH), a cancer stem cell biomarker, is related to drug resistance. Co-treatment of anti-cancer drug (camptothecin: CPT) and ALDH inhibitor (DEAB) can overcome the drug resistance of cancer stem cells (CSCs) and finally cure cancer without relapse. We first introduce a prodrug (DE-CPT) consisting of 1,3-oxathiolane as a reactive oxygen species (ROS) responsive scaffold and an aldehyde protecting group of DEAB to deliver the CPT and DEAB upon delivery reaction with ROS. From the test of sphere-forming ability and CSCs markers subpopulation, we found that the prodrug (DE-CPT) efficiently decreases the CSCs population and kills the cancer cells.



Poster Presentation : **ORGN.P-519**

Organic Chemistry

Event Hall FRI 11:00~13:00

Installation of Ammonium Groups in Metal-Organic Frameworks for Anion Conductivity Study

Seungpyo Hong, Minyoung Yoon[1,*], Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea

[1]*Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea*

Metal-Organic Frameworks (MOFs) are merging porous materials for various applications such as molecular separation, sensing, and catalysis. The organic functional groups in MOFs could be installed into MOFs for target functionalizations. For example, a variety of acidic functional groups has been installed into MOFs for proton conduction study in recent. Carboxylic acid, surfonic acids, and heterocycles were incorporated into MOFs to enhance proton conductivity in the channel of MOFs.[1] The proton conductive MOFs have been applied to membrane material for fuel cell system.

At the same time, the hydroxide conductivity could be considered in MOF's channel.[2] In this case, the positively-charged MOFs are necessary, and the positively-charged functional groups with negative counter ions should be installed in the organic ligand of MOFs.

Recently, we have successfully installed a quaternary ammonium group on tertiary amine-functionalized Zn-based MOFs.[3] However, due to poor water-stability of Zn-based MOFs, this system cannot be utilized in hydroxide conductivity study. Therefore, we have developed that quaternary ammonium groups incorporated Zr-based MOFs for hydroxide conductivity. Both ammonium groups in aliphatic chain and aromatic ring were prepared, and two post-synthetic methods (modification and exchange) have been investigated to efficient installation of ammonium group into MOFs. The detail synthetic procedures and their results will be discussed in the presentation.

References

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Poster Presentation : **ORGN.P-520**

Organic Chemistry

Event Hall FRI 11:00~13:00

Vinyl groups in metal-organic frameworks for covalent connections

Jooyeon Lee, Wonjune Yeo[1], Myungeun Seo[1,*], Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Metal-Organic Frameworks (MOFs) are emerging porous crystalline materials for various applications including molecular separations, energy storage and catalysis. The major feature of these organic-inorganic hybrid material is functional group installation on their strut of framework (i.e., organic ligand of materials). The organic functional groups in MOFs allow the target functionalizations such as carbon dioxide capture through amino group and sulfonic acid group for proton conductivity. In addition, the additional characteristics could be installed in MOFs through organic functional group.

Recently, we have successfully installed vinyl groups into MOFs for further polymerization applications. Since MOFs are crystalline materials, their processability to real applications are quite restricted due to their fragility. Therefore, the physical mixture between MOFs and mixed matrix membranes (MMMs) have been extensively studied to overcome fragile characters. Additionally, we developed the covalent connections between MOFs and MMMs through vinyl groups.

In the first study, we have successfully demonstrated that the covalent connection between MOFs and MMMs through thiol-ene photo-polymerization.[1] The installation of vinyl group prevented the aggregation of MOF particles during polymerization process to form thin film. In addition, the core-functionalizations have been combined with the covalently connected MOF-MMM composite materials. Since the organic functional group installations are important features of MOFs, we have introduced the secondary functional groups in the core part of MOFs through post-synthetic ligand exchange (PSE) technique, then the covalent connections between MOFs and MMMs were performed with vinyl group.[2] Lastly, the assembly of MOFs and porous polymers have been achieved through vinyl-functionalized MOFs. After introducing two polymers on the surface of MOFs, the selective removal of a sacrificial polymer allowed pore-accessible, hierarchical MOF-polymer composite materials. These three studies successfully demonstrated the efficiency and utility of vinyl functional groups in MOFs toward composite material synthesis.

References

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Poster Presentation : **ORGN.P-521**

Organic Chemistry

Event Hall FRI 11:00~13:00

TEMPO-Functionalized MOFs for Selective Aerobic Oxidation of Alcohols

Jonghyeon Lee, Yoonji Heo, Seungpyo Hong, Jooyeon Lee, Houng Kang[1,*], Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea

[1]*Department of Chemistry Education, Chungbuk Natioanl University, Korea*

TEMPO ((2,2,6,6-tetramethylpiperidin-1-yl)oxyl) radical is a stable aminoxyl radical, and has been widely applied to various organic reactions due to their unique radical reactivity. Moreover, their six-membered piperidine core could be modified with other functional groups for further modifications. Recently, we have successfully installed the TEMPO moiety into metal-organic frameworks (MOFs) to apply these radical-functionalized MOFs to various catalytic applications. In general, the TEMPO radicals have been utilized in aerobic oxidation system, especially for aerobic oxidation of alcohols to corresponding aldehyde. Therefore, we have applied TEMPO-functionalized MOFs to aerobic oxidation of alcohols to aldehyde under mild condition. In specific, the secondary redox cycles were required, and the Eu(II)/Eu(III) cycles were combined with TEMPO functional group in MOFs to maximize their catalytic activity to aerobic oxidation.[1]

In addition, the surface deactivation strategy was successfully demonstrated in TEMPO-functionalized MOFs (UiO-67-TEMPO) to achieve the substrate size selectivity on aerobic oxidation. After deactivating (removing) TEMPO species on the surface of MOFs, the substrate must be penetrated into MOF pore to meet TEMPO radical. Therefore, the large substrate than pore size of MOFs cannot be oxidized under the surface-deactivated, TEMPO-functionalized MOFs.[2]

Lastly, the sequential two-step oxidation of alcohols to carboxylic acids were successfully achieved TEMPO-functionalized MOFs (UiO-68-TEMPO). Since the autooxidation of aldehydes to carboxylic acids were totally halted under TEMPO condition, we needed to develop ‘MOF-in-and-out’ method to control the existence of TEMPO species in the solution mixture. The first aerobic oxidation was performed with MOF (MOF-in) and the following autooxidation of aldehyde to carboxylic acid was occurred without MOF

(MOF-out).[3] A series of our studies successfully demonstrated the unique feature of TEMPO-functionalized MOFs to catalytic organic reactions. The detail studies will be presented with summarized results and direct comparisons.[4]

References

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Poster Presentation : **ORGN.P-522**

Organic Chemistry

Event Hall FRI 11:00~13:00

2D-Ultrathin MXene/DOXjade Platform for Iron Chelation Chemo-photothermal Therapy

Yunjie Xu, Jusung An, Mingle Li, Ji Hyeon Kim, Ilwha Kim, Yuvin Noh, Subin Son, Byungkook Kim, Minhyeok Choi, Jongseung Kim*

Department of Chemistry, Korea University, Korea

An increased demand for iron is a hallmark of cancer cells and is thought necessary to promote high cell proliferation, tumor progression and metastasis. This makes iron metabolism an attractive therapeutic target. Unfortunately, current iron-based therapeutic strategies often lack effectiveness and can elicit off-target toxicities. We report here a dual-therapeutic prodrug, DOXjade, that allows for iron chelation chemo-photothermal cancer therapy. This prodrug takes advantage of the clinically approved iron chelator deferasirox (ExJade®) and the topoisomerase 2 inhibitor, doxorubicin (DOX). Loading DOXjade onto ultrathin 2D Ti_3C_2 MXene nanosheets produces a construct, Ti_3C_2-PVP@DOXjade, that allows the iron chelation and chemotherapeutic functions of DOXjade to be photo-activated at the tumor sites, while potentiating a robust photothermal effect with photothermal conversion efficiencies of up to 40%. Antitumor mechanistic investigations reveal that upon activation, Ti_3C_2-PVP@DOXjade serves to promote apoptotic cell death and downregulate the iron depletion-induced iron transferrin receptor (TfR). A tumor pH-responsive iron chelation/PTT/chemotherapy antitumor effect was achieved both in vitro and in vivo. The results of this study highlight what may constitute a promising iron chelation-based phototherapeutic approach to cancer therapy.

Poster Presentation : **ORGN.P-523**

Organic Chemistry

Event Hall FRI 11:00~13:00

Conditionally Activatable Photoredox Catalysis in Living Systems

Mingle Li, Yunjie Xu, Ilwha Kim, Subin Son, Yuvin Noh, Jusung An, Ji Hyeon Kim, Saehee Rha, Jieun Lee, Jongseung Kim*

Department of Chemistry, Korea University, Korea

The transformational impact of photoredox catalytic chemistries has inspired new opportunities enabling us to interrogate nature in ways that are not possible otherwise and to unveil new biotechnologies in therapy and diagnosis. However, the deployment of artificial photoredox catalysis in living systems remains challenging, mired by the off-target risk and safety concerns of photocatalyst toxicity. Here, we present an appealing approach, namely conditionally activatable photoredox catalysis (ConAPC), and as proof of concept design the first ConAPC architecture (Se-NO2) based upon classic self-immolative chemistry, in which the inherent photocatalytic properties can be temporarily caged while become active only at the tumor sites via sensing to specific biomarkers. Such masking strategy allows a spatial-temporal control of photoresponsivity in vitro and in vivo. In particular, for ConAPC design, a new biologically benign metal-free photocatalyst (Se-NH2), which is able to initiate NIR photoredox catalysis to manipulate cellular electron pool in an O2-independent mechanism of action, is identified. With this unique strategy, potent tumor-specific targeting photocatalytic eradication (TGI: 95%) is obtained in mouse model. Impressively, favorable features such as high-resolution tumor recognition (SBR: 33.6), excellent biocompatibility and safety are also achieved. This work therefore offers a new possibility for chemists to leverage artificial photocatalytic reactions toward the development of facile and intelligent photocatalytic theranostics.

Poster Presentation : **ORGN.P-524**

Organic Chemistry

Event Hall FRI 11:00~13:00

Alkenylation of Allene C(sp2)–H Bonds with a Palladium Catalyst

Mina Son, Benedikt Schreib[1], Francoise Aouane[1], Mu-Hyun Baik[*], Erick Carreira[1,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*ETH Zurich, Switzerland, Switzerland*

While a number of C–H bond activations have been reported for the aliphatic, aromatic, alkene, and alkyne substrates, the same approach has not been reported for the allenyl substrates, largely due to the reactive internal carbon within the alleneyl scaffold. Computational studies show the internal carbon activation can be hindered with the use of bulky functional groups. Using a picolinamide as a directing group and using a sterically demanding functional group, activation of allene C(sp^2)–H bonds and subsequent alkenylation is achieved. Density functional theory(DFT) studies provide a detailed mechanistic pathway, in which the initial C–H bond is activated through a concerted metallation-deprotonation step. Also, the rate-determining step is suggested to be the beta-hydride elimination step, which is in line with the experimental studies.

Poster Presentation : **ORGN.P-525**

Organic Chemistry

Event Hall FRI 11:00~13:00

Single-Benzene Dual-Emitters: Harnessing Excited-State Antiaromaticity to Generate White-Light with a Small Molecule

Younghun Kim, Heechan Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Small-sized light-emitters suffer less from inter- or intramolecular interactions than conventional π-extended fluorophores. In the solid-state and biological environment, this property becomes even more advantageous. For a small π-conjugation to emit visible light, a large Stokes shift is an important prerequisite. Single-benzene fluorophores (SBFs) are ideal candidates as they are built on the small benzene core yet exhibit large Stokes shifts by relieving the excited-state antiaromaticity (ESAA). Several SBFs have been developed with impressive photophysical properties, but dual-emissive SBFs are currently unknown. Knowing that benzene derivatives can take various pathways to alleviate ESAA, we decided to harness the ESAA of SBF to implement two different radiative pathways to realize dual emission. For this purpose, two pairs of amide and acetyl groups were embedded in a benzene core as electron donors and acceptors while simultaneously serving as hydrogen bonding donor and acceptor pairs for excited-state intramolecular proton transfer (ESIPT). A series of dual-emissive SBFs were prepared by systematically increasing the acidity of the amide N–H group to finely modulate the excited-state energetics of proton transfer reaction. Remarkably, an adequate balance of ESIPT equilibrium produces white light in both solution and solid-state. Our theoretical analysis suggests that structural relaxation to strengthen two pairs of intramolecular hydrogen bonds of the locally excited state and the complete transfer of a single proton in the ESIPT state are both responsible for the relief of ESAA. This presentation will discuss a new strategy for developing single-molecule dual-emitters and their applications in white light-emitting devices and perfluorocarbon nanodroplets.

Poster Presentation : **ORGN.P-526**
Organic Chemistry
Event Hall FRI 11:00~13:00

A novel temozolomide analog for overcoming MGMT-mediated drug resistance in glioblastoma

Ilwha Kim, Jusung An, Subin Son, Ji Hyeon Kim, Yuvin Noh, Byungkook Kim, Saehee Rha, Minhyeok Choi, Zehra Zunbul[1], Jongseung Kim[*]

Department of Chemistry, Korea University, Korea
[1]*Chemistry, Korea University, Korea*

Glioblastoma (GBM; grade IV astrocytoma) is the most common primary malignant brain tumor that originates from astrocytes. The global incidence of GBM is 3.19 per 100,000 people, and the median survival period is only 15 months after diagnosis. Currently, widely recognized treatments in GBM include surgery, radiation, and chemotherapy. Temozolomide (TMZ), the first-line treatment for GBM, is a DNA alkylating agent that can easily penetrate the BBB since it's a lipophilic agent. It alkylates N^7 and O^6 positions of guanine and N^3 sites of adenine which lead to apoptosis.However, TMZ-resistance associated with O^6-methylguanine-DNA methyltransferase (MGMT) is a significant limitation of GBM treatment. MGMT is a DNA repair enzyme that removes the alkyl group in O^6-methylguanine (O^6-MeG), the primary cytotoxic DNA lesion induced by TMZ. Thus, MGMT inhibitors (such as lomeguatrib) are an essential anticancer therapeutic approach to overcome TMZ resistance.Herein, a small-molecule lomeguatrib-conjugated TMZ analog (TA1) that can circumvent TMZ resistance and achieve therapeutic effects at the same time was designed for treating glioblastoma.

Poster Presentation : **ORGN.P-527**

Organic Chemistry

Event Hall FRI 11:00~13:00

Approach to α,β-unsaturated ketones through nickel catalyzed aldehyde-free hydroacylation

Jeong woo Lee, Sung You Hong*

Chemistry, Ulsan National Institute of Science and Technology, Korea

α,β-Unsaturated ketones are widely used as raw materials in the production of fine chemicals, medicines, and natural products. Through chemoselective aldehydic C–H activation, transition metal-catalyzed hydroacylation processes of alkynes employing aldehydes have been recognized as an atom-economical method to access, unsaturated ketones. However, chelating moiety-bearing aldehydes are required in previously described hydroacylation reactions utilizing rhodium, cobalt, or ruthenium catalysts to prevent decarbonylation of acyl-metal-hydride complexes. In the presence of zinc metal as a reducing agent, we present a nickel-catalyzed anti-Markovnikov selective coupling process that yields non-tethered E-enones from terminal alkynes and S-2-pyridyl thioesters. This method, which is not chelation-controlled, has mild reaction conditions and excellent regio- and stereoselectivity.

Poster Presentation : **ORGN.P-528**

Organic Chemistry

Event Hall FRI 11:00~13:00

Air-, Moisture-Tolerant Nickel Catalysis and Regioselective Synthesis of Multi-Substituted Pyridines

Jihwan Jeon, Sung You Hong*

chemistry, Ulsan National Institute of Science and Technology, Korea

Nickel(0)-catalyzed [2+2+2] cycloaddition reaction of 1,6-diynes and nitrile has been limited to air and moisture sensitive Ni(COD)2 system. Here in, we studied air and moisture sensitive Ni(0) system through in situ generation of Ni-Xantphos species. Our system afforded the complementary regioisomers. The origin of the regioselectivity was explained by frontier molecular orbital interactions with DFT calculation.

Poster Presentation : **ORGN.P-529**

Organic Chemistry

Event Hall FRI 11:00~13:00

Nickel-catalyzed Chemo- and Regioselective Azide–Alkyne Cycloaddition

SeoYeong Jeong, Sung You Hong*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

The metal-catalyzed cycloaddition is straightforward pathway to make functionalized heterocyclic frameworks. It has been challenging to achieve reactivity-controlled metal-catalyzed azide–alkyne cycloadditions for chemoselectivity of internal alkynes. In this paper, we describe a nickel-catalyzed [3 + 2] cycloaddition of unsymmetrical alkynes with azides that forms functionalized 1,2,3-triazoles with excellent regio- and chemoselectivity. For the clarification of the reaction mechanism, Density functional theory calculations are utilized. The computed mechanism shows that the oxidative addition of the alkyne substrate to the Ni(0)–Xantphos catalyst, followed by C–N coupling of the nickellacyclopropene intermediate, produces a nickellacyclopropene intermediate. And the consequent C–N coupling of this intermediate with an azide is responsible for the chemo- and regioselectivity.

Poster Presentation : **ORGN.P-530**

Organic Chemistry

Event Hall FRI 11:00~13:00

Narrowing Band Gap of Polydopamine Nanoparticles by an Amyloid Scaffold

Yu jin Kang

applied chemistry, Kyung Hee University, Korea

Nanoparticles of polydopamine and its derivatives are recently being used as a versatile photoreactive material. Akin to melanin, a natural pigment, polydopamine nanoparticles exhibit many interesting physicochemical features, including broad light absorption, stable radical character, and an efficient photothermal conversion property. Inspired by biological melanogenesis, where amyloid fibers play central roles as a functional scaffold, we asked whether using amyloid scaffolds for the synthesis of polydopamine nanoparticles could modulate (or enhance) their materials properties. By using cyclic voltammetry, electron paramagnetic resonance spectroscopy, and other analytic tools, we showed that the presence of amyloid scaffolds narrowed the band gap of polydopamine nanoparticles critically, which concomitantly improved their radical scavenging capability and efficiency of photothermal conversion.

Poster Presentation : **ORGN.P-531**

Organic Chemistry

Event Hall FRI 11:00~13:00

Direct and Regioselective Pd(II)-Catalyzed B(4)−H Monoacyloxylation and B(4,5)−H Diacetoxylation of *o*-Carborane Acids with Phenyliodonium Dicarboxylates

Kyungsup Lee, Hee Chan Noh, Phil Ho Lee*

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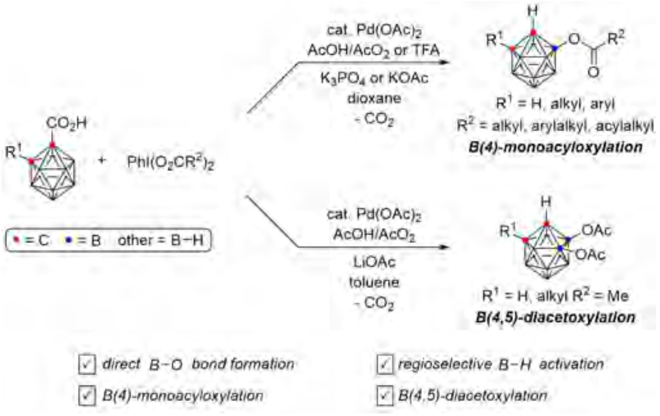
The regioselective introduction of a functional group onto *o*-carboranes has received considerable attention because of its potential applications in boron neutron capture therapy (BNCT), medicinal chemistry, optoelectronic functional materials, supramolecular/coordination chemistry, and catalysis. In contrast to the introduction of a carbon-functional group onto cage boron of *o*-carboranes, the introduction of a heteroatom-functional group onto a cage boron is comparatively less explored. Moreover, in spite of the omnipresent existence of B−O bonds in borates, boron esters, and boric acids, the introduction of an oxygen functional group onto a cage boron of *o*-carboranes has not been well-investigated. Consequently, the development of a mild and efficient method for the direct and regioselective construction of a B−O bond via a B−H functionalization is still a challenging subject. In a continuation with our studies directed toward the development of a transition-metal catalyzed functionalization of *o*-carboranes, we demonstrate herein a direct and regioseletive Pd-catalyzed B(4)-monoacyloxylation and B-(4,5)-diacetoxylation reaction of *o*-carborane acids with phenyliodonium dicarboxylates.



Poster Presentation : **ORGN.P-532**

Organic Chemistry

Event Hall FRI 11:00~13:00

One-pot sulfa-Michael addition reactions using disulfides under visible-light irradiation

Changhee Park, Sunggi Lee[1,*]

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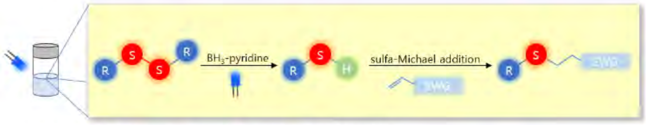
The organic sulfur compound is one of the most important compounds in the synthesis of natural and pharmacological compounds. The general method for the synthesis of the C-S bonds utilizes odorous and toxic thiols as starting materials. As alternatives, odorless, low-toxic, air-stable disulfides have been employed. However, the generation of thiol from disulfide requires strong reducing agents or transition metals resulting in low functional group tolerance or high toxicity issues. For these reasons, it is necessary to develop a new method that reductive cleavage of disulfide to thiol under transition metal-free and mild conditions. Herein, we report the new reduction method that converts disulfides to the corresponding thiols and enables one-pot sulfa-Michael addition reactions using the borane-pyridine complex as a mild reducing agent, under the irradiation of blue light without transition metal. This novel synthetic approach provides significant advantages in terms of broad substrate scope, functional group tolerance, and economic benefits.



- Reduction of disulfides to the corresponding thiols under mild condition
- One-pot sulfa-Michael addition
- Transition metal free

Poster Presentation : **ORGN.P-533**

Organic Chemistry

Event Hall FRI 11:00~13:00

Meta-selective C-H Functionalization of Arenes using Silicon Tether

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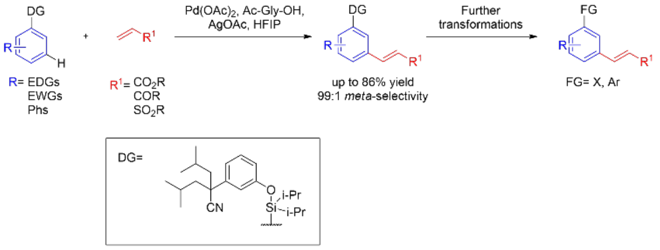
Regioselective C-H functionalization in aromatic compounds with the directing group has been studied in the last several decades. While proximal ortho-functionalization is well known, distal meta- or para-functionalization is more challenging. Our group developed direct meta-selective C-H alkenylation via palladium catalyst with the silicon-containing directing group, which is readily introduced and removed at the same time synthesized in two steps. The bulkiness of alkyl groups on alpha-methylene to nitrile was enabled to control selectivity by changing the direction of nitrile group. When iso-butyl group was introduced, the highest meta-selectivity was obtained. Using this directing group, olefinated products were prepared with good to excellent selectivities regardless of the electronic nature of substituted arenes. Interestingly, when polyaromatics were employed, one of several C-H bonds was functionalized with moderate selectivities. Various olefins next to ketone, sulfone, and esters also afforded desired products with high meta-selectivities. Furthermore, by transforming the silicon directing group into other functional groups like deuterium and halide, tri-substituted arenes were synthesized efficiently. Finally, Hiyama-Denmark cross-coupling reaction after meta-selective C-H alkenylation gave the biaryl structure.



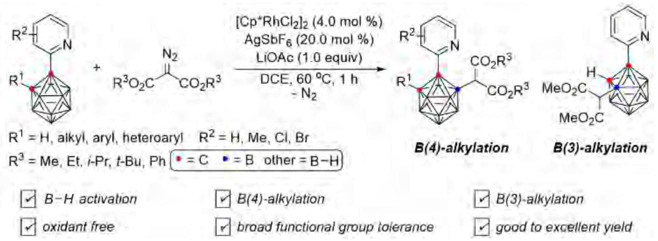
Poster Presentation : **ORGN.P-534**
Organic Chemistry
Event Hall FRI 11:00~13:00

Rhodium-Catalyzed B(4)−H and B(3)−H Alkylation Reaction of Pyridyl *o*-Carboranes with Diazodicarboxylates

Gi Hoon Ko, Hee Chan Noh, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Carboranes are a kind of clusters composed of carbon and boron having three-dimensional aromaticity (σ-aromaticity) as analogs of two-dimensional benzenes (π-aromaticity). These compounds have distinctive characteristics, such as aromaticity and high chemical stability, and are found in many applications, including boron neutron capture therapy, supramolecular design, coordination/organometallic chemistry, fluorescence/phosphorescence, and materials science. These special properties and interesting applications have received considerable attention to functionalize carboranes. Recently, transition metal-catalyzed B−H activation has emerged as an effective method for regio- and stereo-selective functionalization of *o*-carboranes and has resulted in great progress. However, because reactivity of ten BH bonds in *o*-carboranes are not equal, the regioselective introduction of functional group onto *o*-carboranes is still difficult. Accordingly, site-selective and effective functionalization of *o*-carboranes is an ongoing challenge. We demonstrated a streamlined Rh-catalyzed B(4)−H and B(3)−H alkylation reaction of a variety of pyridyl *o*-carboranes with *α*-diazomalonates via B−H activation with the evolution of nitrogen gas.



Poster Presentation : **ORGN.P-535**

Organic Chemistry

Event Hall FRI 11:00~13:00

Pd-Catalyzed *N*-Carbonylative Cross-Coupling Reaction of Sulfoximines with Aryl, Heteroaryl, and Alkenyl Halides Using Tungsten Hexacarbonyl as Carbon Monoxide Source

Sang Hoon Han, Hee Chan Noh, Phil Ho Lee*

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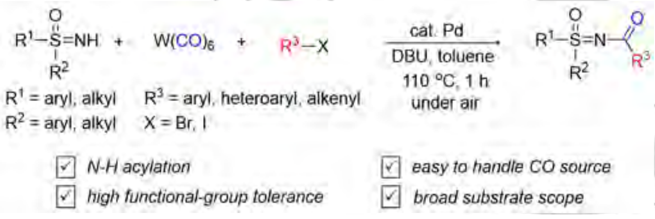
Palladium(II)-catalyzed *N*-acylation was demonstrated through the reaction of N−H sulfoximines with a variety of aryl, heteroaryl, and aryl halides using $W(CO)_6$ as a source of carbon monoxide, affording *N*-acylated sulfoximines in good to excellent yields. Moreover, alkenyl bromides underwent palladium(II)-catalyzed *N*-acylation reactions with N−H sulfoximines, leading to the formation of *N*-cinnamoyl sulfoximines. This method has the advantages of a broad substrate scope, high functional group tolerance, simple operation, and chemoselectivity between chloride and bromide.



Poster Presentation : **ORGN.P-536**

Organic Chemistry

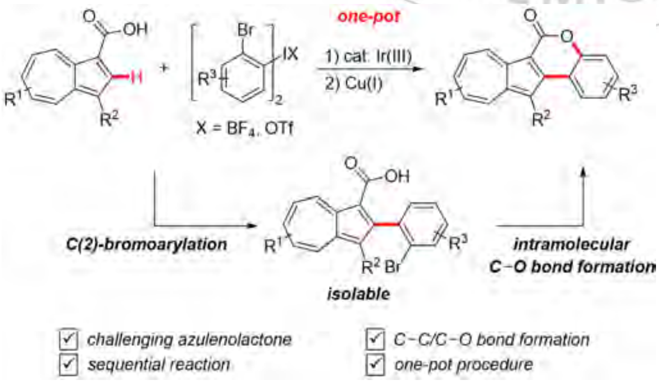
Event Hall FRI 11:00~13:00

Synthesis of Azulenolactones through Sequential C(2)-Bromoarylation and Intramolecular C−O Bond Formation from Azulene-1-carboxylic Acids and Di(2-bromoaryl)iodonium Salts in One Pot

Chanyoung Maeng, Hee Chan Noh, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Azulene, as a representative compound of nonbenzenoid aromatic hydrocarbons, has received much attention due to its importance in natural products, functional materials, and biologically active compounds. Accordingly, the establishment of a streamlined synthetic approach for azulene skeletons from easily obtainable starting materials is extremely important. In particular, as the 2-position of azulene is less nucleophilic than the 1,3-position, the introduction of substituents to the 2-position remains a challenge in organic synthesis. we have demonstrated an iridium(III)-catalyzed C(2)-bromoarylation reaction followed by copper(I)-mediated intramolecular C−O bond formation from azulene-1-carboxylic acids and di(2-bromoaryl)iodonium salts in one pot, resulting in the formation of azulenolactones. The sequential reaction proceeded smoothly via Cu(I)-mediated cyclization of 2-(2-bromoaryl)azulene-1-carboxylic acids derived from the regioselective iridium(III)-catalyzed C(2)-bromoarylation reaction without decarboxylation.



Poster Presentation : **ORGN.P-537**

Organic Chemistry

Event Hall FRI 11:00~13:00

Photocatalytic endomembrane oxidation triggers pyroptotic cell death

Chaiheon Lee, Mingyu Park, Tae-Hyuk Kwon[1,*]

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[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Programmed cell death is an essential function encoded within cells that maintaining homeostasis of organism by eliminating cells which are irreversibly damaged or potentially harmful. Pyroptosis, a lytic programmed cell death, is an influential signal to induce intense inflammatory and immune response; manipulating pyroptotic cell death is a prerequisite for releasing immunogens in medical uses. However, the biochemical methods initiating pyroptotic cell death at the desired spatiotemporal point and their principles are unknown, which complicates elucidating unclear part of the pyroptosis mechanism as well as applications to the clinical field. Here, we show photocatalytic endomembrane oxidation triggers gasdermin activation and subsequent pyroptotic cell death. The endomembrane-localised organic photosensitiser, BTP, selectively generates hydroxyl radicals from water and visible light. The produced hydroxyl radicals cause severe oxidative stress to endomembrane including membrane proteins and unsaturated lipids, accumulating misfolded membrane proteins. The proteomic analysis shows membrane proteins related to unfolded protein response (UPR), ER-Golgi transport, mitochondrial translation, and lipid metabolism are significantly oxidised. The single protein force microscopy technique reveals that the oxidation damages folding abilities by breaking down secondary/tertiary structure of membrane proteins. As a results of accumulation of misfolded proteins, the cells exhibit maladaptive unfolded protein responses (UPR), leading to caspase-induced gasdermin d activation.

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Poster Presentation : **ORGN.P-538**

Organic Chemistry

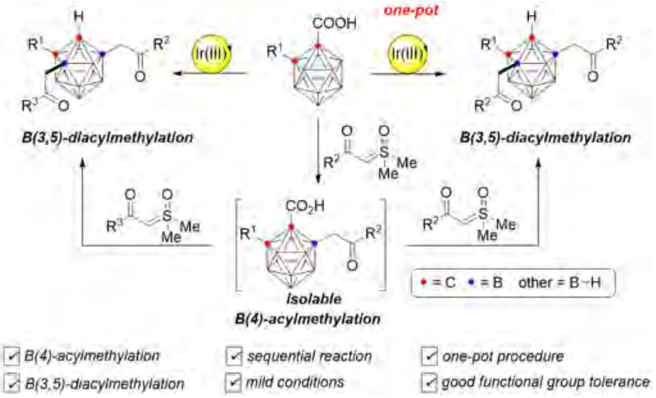
Event Hall FRI 11:00~13:00

Iridium(III)-Catalyzed B(4)-Acylmethylation and B(3,5)-Diacylmethylation from *o*-Carboranes and Sulfoxonium Ylides

Hee Chan Noh, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

Carboranes, a kind of three-dimensional cluster of benzene, have demonstrated as functional skeletons in boron neutron capture therapy (BNCT) agents, in building blocks in nanomaterials, and in versatile ligands for transition metals. Accordingly, functionalization of carboranes has received much attention, and then a large number of approaches have been reported for the functionalization of cage CH and BH vertexes to date. Generally, because the cage BH proton is less acidic than that of the cage CH proton (pKa ~ 23), cage B−H activation followed by functionalization is difficult compared to that of C−H ones. In addition, since ten BH vertexes are on the carborane, it is much more difficult to control regioselectivity of ten BH vertexes compared to two CH vertexes. Thus, the establishment of efficient method for the introduction of a broad range of functional groups to BH vertexes of carboranes is very fascinating and challenge. Described herein is the first Ir-catalyzed cage B(4)-acylmethylation reaction of *o*-carboranes with sulfoxonium ylides by carboxylic acid-assisted B(4)−H bond activation under extremely mild conditions, producing B(4)-acylmethylated *o*-carboranes and B(3,5)-diacylmethylated *o*-carboranes through sequential B(4)- and B(6)-acylmethylation reaction in one pot.



Poster Presentation : **ORGN.P-539**

Organic Chemistry

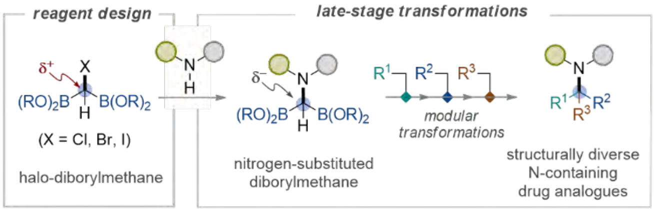
Event Hall FRI 11:00~13:00

Diborylmethyl Group as a Transformable Building Block for the Diversification of Nitrogen-Containing Molecules

Chiwon Hwang, Seung Hwan Cho*

Department of Chemistry, Pohang University of Science and Technology, Korea

The discovery of new strategies for the formation and manipulation of C(sp3)-N bonds has long been of great interest, since a myriad of pharmaceuticals, agrochemicals and biologically active compounds contain nitrogen functionalities. Over the past several decades, representative methods, including nucleophilic substitution with alkyl electrophiles, reductive amination, TM-catalyzed C-N cross-coupling of organohalides, hydroamination of alkenes and C-H amination reactions, have been well established as suitable approaches for constructing C(sp3)-N bonds. Nevertheless, the effectiveness of each of these reactions is strongly dependent on the substrates and/or reaction conditions, thus often requiring additional optimization(s) to be applicable in late-stage functionalizations of complex molecules. Moreover, the synthesis of structurally interesting drug analogues would entail parallel and laborious synthetic efforts in addition to the mentioned reactions. In order to introduce diverse carbon motifs onto a nitrogen functionality, especially those embedded in naturally abundant and synthetic bioactive molecules, a potentially powerful strategy would be to first insert a universally transformable carbon moiety in an N-H functionality to yield an intermediate that could be converted to other synthetically valuable motifs, whenever necessary, in a predictable and programmable manner.In this presentation, we describe an unprecedented method for the preparation of a-amino-diborylmethanes through homologative coupling between a-halo-diborylmethanes and nitrogen nucleophiles. This process shows a remarkably broad substrate scope, and the usefulness of the developed method is exemplified in the late-stage diversification of nitrogen-containing biologically relevant molecules.


reagent design
late-stage transformations
δ+
X
(RO)2B
B(OR)2
H
(X = Cl, Br, I)
halo-diborylmethane
N
H
δ−
N
(RO)2B
B(OR)2
H
nitrogen-substituted
diborylmethane
R1
R2
R3
modular
transformations
N
R1
R2
R3
structurally diverse
N-containing
drug analogues

Poster Presentation : **ORGN.P-540**

Organic Chemistry

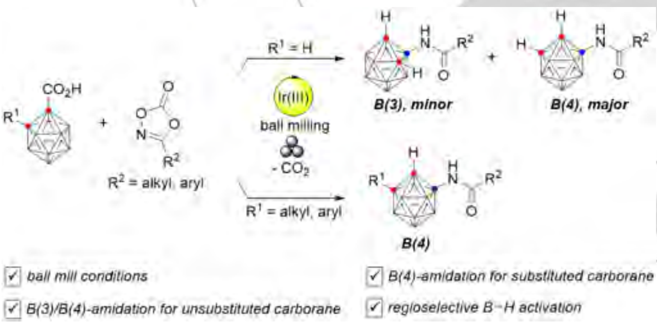
Event Hall FRI 11:00~13:00

Mechanochemical Ir(III)-Catalyzed B-Amidation of *o*-Carboranes with Dioxazolones

<u>Gi Uk Han</u>, Hee Chan Noh, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Mechanochemistry was successfully applied to the functionalization of carboranes. Mechanochemical iridium(III)-catalyzed regioselective B(3)- and B(4)-amidation of unsubstituted *o*-carboranes with dioxazolones have been developed. In addition, mechanochemical iridium(III)-catalyzed regioselective B(4)-amidation of substituted *o*-carboranes was demonstrated. Since mechanochemical B-amidation proceeds smoothly without organic solvents and external heating, the present method is regarded as a sustainable and environmental-friendly surrogate for typical solvent-based reactions.



Poster Presentation : **ORGN.P-541**

Organic Chemistry

Event Hall FRI 11:00~13:00

Cu(I)-Catalyzed Enantioselective [5 + 1] Cycloaddition of N-Aromatic Compounds and Alkynes via Chelating-Assisted 1,2-Dearomative Addition

Changjin Oh, Eun Jeong Yoo[1,*], Mu-Hyun Baik[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Copper-catalyzed [5 + 1] cycloadditions of Naromatic zwitterions have been accomplished by chelation-assisted 1,2-dearomative addition of electron-deficient terminal alkynes. The unique modular skeleton of pyrazino[1,2-a]quinoline could be obtained from the regio-and stereoselective cascade annulation process, which was supported by computational studies. Further, an asymmetric variant of the developed strategy has been successfully extended for enabling access to optically enriched six-member cyclic systems.

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Poster Presentation : **ORGN.P-542**
Organic Chemistry
Event Hall FRI 11:00~13:00

Controlling the equilibrium of dynamic chemistry by amyloid's functional residue

Sehui Yoo

Applied chemistry, Kyung Hee University, Korea

Although amyloid has been considered as a pathological factor for a long time, functional amyloid nowadays is getting much interest as a biological nanomaterial with various applications. In some ways, amyloid structure can be used as template to present functional residue out of surface and can catalyze various chemical reactions. Herein, we design peptide residue which self-assemble into amyloid fibrils to control equilibrium of reversible chemical reactions that widely used in dynamic covalent chemistry. Also we investigate the relationship between the kind of functional residue and catalytic ability in dynamic covalent reactions. This study have meanings in not only a discovery of de novo functionality of amyloid but also a great potential for developing to effective biocatalysts.

Poster Presentation : **ORGN.P-543**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fmoc-amino acid as a minimal molecular scaffold for liquid-liquid phase separation

Joohyung Lee

Applied Chemistry, Kyung Hee University, Korea

Liquid-liquid phase separation (LLPS) is associated with most cellular processes, including stress response, signal transduction, gene expression, and protein aggregation. Its molecular level-mechanism(s), however, remains incompletely understood. A set of minimal molecular scaffolds with which LLPS can be systematically studied would be greatly useful for both understanding and utilizing LLPS. In this study, we investigated LLPS behaviors of Fmoc-protected amino acids. Fmoc-amino acids have long been studied for their fibrogenetic behaviors, but their LLPS has not been reported yet. We found that a large portion of Fmoc-amino acids exhibit LLPS phenomenon, depending on pH and ionic strength of the solution. We systematically asked the conditions in which each Fmoc-amino acid undergoes LLPS, and demonstrated that liquid coacervates made of Fmoc-amino acids can be useful for various enrichment of biomolecules or catalysis of organic reactions.

Poster Presentation : **ORGN.P-544**

Organic Chemistry

Event Hall FRI 11:00~13:00

The Mechanism behind Enhanced Reactivity of Substituted Ethynyl Phosphonate Electrophiles towards Thiols

Dongju Kim, Christian E. Stieger[1], Christian P.R. Hackenberger[1,*], Mu-Hyun Baik[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Chemical Biology Department, Leibniz-Forschungsinstitut fűr Molekulare Pharmakologie, Germany*

Site-selective chemical functionalization of proteins provides the possibility to probe and alter their biological function. Recently reported diethynyl phosphinates are thiol reactive reagents suitable for cysteine-selective protein functionalizations. However, the reaction rate of thiovinyl-substituted ethynyl phosphonates was lower than the non-substituted diethynyl phosphinates. The prolonged handling times might be disadvantageous for some proteins. To address this issue, we benchmarked various substituents using DFT calculations. Triazoyl-substituted ethynyl phosphonates were selected for easily accessed and highly reactive electrophiles towards thiols for protein functionalization. The inductive effect and π-conjugation were key factors in increasing the reaction rate of ethynyl-phosphonates. Electron-withdrawing effect of triazole substituent makes terminal carbon more electrophilic. The π-bonding between the central P-atom and triazole lowers the P-atomic orbitals to accept the lone pair of the generated carbanion in the vicinal position. Based on these results, cysteine-selectivity and superior reaction kinetics were demonstrated through various experiments. Our study provides the possibility of widespread application of diethynyl-phosphinates for protein functionalizations.

Poster Presentation : **ORGN.P-545**

Organic Chemistry

Event Hall FRI 11:00~13:00

Ligand-divergent Double Hydroboration of Pyridines by the Rhodium Catalyst

Hyoju Choi, Ruibin Wang[1], Sehoon Park[1,*], Mu-Hyun Baik[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Chemistry, Guangdong Technion Israel Institute of Technology, China*

Catalytic hydroboration is a competent method with advantages such as mild reaction conditions, easy-to-handle and variable reducing agents, and good functional group tolerance. Chemo- and regio-selective hydroboration of N-heteroarenes is a highly desired reaction path, leading to di- or tetrahydropyridine derivatives from the parent pyridine molecules. Recently, our group and Park group have actively studied ligand-divergent double hydroboration of pyridine by the rhodium catalyst. We have found that 2nd Hydroboration using the PPh_3 ligand easily occurs within a short time. On the other hand, 2nd Hydroboration using PCy_3 ligand is obstructed, leading to dihydropyridine as a major product. To reveal the full reaction mechanism and the key factors at the ligand-divergent double hydroboration, detailed mechanistic study by density functional theory calculations and experimental methods are ongoing.

Poster Presentation : **ORGN.P-546**

Organic Chemistry

Event Hall FRI 11:00~13:00

A General Strategy to Enhance Therapeutic Efficiency for Photodynamic/Chemo Synergistic Therapy

Seongman Lee, Songyi Lee[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

Photodynamic therapy and chemotherapy are types of cancer treatment. In this study, we designed a photosensitizer (RL) to achieve the synergy of photodynamic therapy and chemotherapy. RL consists of photosensitizer part with high singlet oxygen quantum yield and prodrug part activated by redox stress (GSH and H_2O_2) in heterogeneous tumors. In solution study, it showed the increased fluorescence at 430 nm by releasement of camptothecin(CPT) under redox stress conditions. And it exhibited good singlet oxygen quantum yield ($\Phi_\Delta = 0.46$) under 530 nm LED irradiation. In vitro, we studied its low dark toxicity in CT26 cells (murine colon cancer cell) by MTT assay. And we expect therapeutic synergy of its photodynamic/chemo therapeutic ability in redox stress environment of heterogeneous tumors. Thus, we suggest the strategy of photodynamic/chemo synergistic therapy, which can increase the therapeutic efficiency of cancer cell.

Poster Presentation : **ORGN.P-547**

Organic Chemistry

Event Hall FRI 11:00~13:00

Restriction of ancillary ligand flexibility enables reducing non-radiative decay pathway for deep-red and NIR emissive iridium(III) complexes

Taehyun Kim, Hae Un Kim, Taiho Park*

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

Deep red and NIR wavelength emissive luminogens have serious quenching problems such as triplet-triplet annihilation and non-radiative decay pathway by the small energy band gap. Moreover, due to the molecular vibration and flexibility accelerate non-radiative energy losses. Herein, we synthesized two novel iridium(III) complexes with phosphorescence property, introducing substituents to main ligands. Electron donating –CH3(Ir1-pic) and -H(Ir2-pic) groups were attached to the N-coordinating quinolone moiety of cyclometalated ligand. In addition, rigid picolinate ancillary ligands were introduced for the restriction of ancillary ligand flexibility. The octahedral coordination and restricted ancillary ligand flexibility enable high triplet energy levels and robust emission. We also deeply analyze the DFT calculations and 2D crystallography in order to investigate photophysical properties. Consequently, Ir1-pic and Ir2-pic showed PLQY values of 0.48 and 0.37, respectively. Solution processed OLEDs based on Ir1-pic and Ir2-pic emitters exhibited maximum EQE values of 5.03% and 3.41%, respectively.

Poster Presentation : **ORGN.P-548**

Organic Chemistry

Event Hall FRI 11:00~13:00

The Synthesis of [^{18}F]Sulfamoyl Fluorides through Late-Stage ^{18}F/^{19}F Isotopic Exchange

Min Pyeong Kim, **Sung You Hong**[1,*]

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Direct [18F]fluorosulfurylation of amines with 1,1-sulfuryl diimidazole did not work well, so the thing finding another pathway to synthesize [^{18}F]sulfamoyl fluoride has been recognized importantly. Here in, we reported that the late-stage ^{18}F/^{19}F isotopic exchange with excellent radiochemical yields. Also, we proposed the efficient protocol *via* automated radiosynthesis, expanding chemical library of sulfamoyl fluorides.

Poster Presentation : **ORGN.P-549**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Self-assembly of the α/β Peptidic Foldamer with Extensive Functional Group

Minsang Kang, Jaewook Kim, Hee-Seung Lee*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Foldecture, a micro-sized 3D structure constructed via non-covalent interaction of peptidic foldamers, has been developed to a variety of shape and sized structure. Previous studies have shown a C_3-symmetrical foldecture with the possibility of supramolecular guest-host interaction. Herein, we attempted to broaden functionality while maintaining structural features of foldecture by replacing the *C*-terminal residue of previously reported α/β peptidic foldamer. We synthesized an 11-helical heptamer, the *C*-terminal residue of which is substituted with aspartic acid, self-assembles to form a three-fold symmetrical bipyramidal shape. In the structural analysis through high-resolution powder X-ray diffraction, we confirmed that the synthesized structure was the same as the previously announced C_3-symmetric fold structure. Successful *C*-terminal residue substitution has shown the potential for the introduction of other monomers such as serine.

Poster Presentation : **ORGN.P-550**

Organic Chemistry

Event Hall FRI 11:00~13:00

Utilizing Maximal Photon Usage of Single-laser-activated Dual Photoactivable Organic Nanotheranostic: Mitochondria-targeted Phototherapeutic Processing for Hypoxic Tumor Treatment

Jinwoo Shin, Yuling Xu[1], Subin Son, Ji Hyeon Kim, Jusung An, Jin yong Lee[2], Amit Sharma[3], Yao Sun[1], Jongseung Kim*

Department of Chemistry, Korea University, Korea
[1]*College of Chemistry, Key Laboratory of Pesticides and Chemical Biology, China*
[2]*Department of Chemistry, Sungkyunkwan University, Korea*
[3]*CSIR-CSIO, Sector 30C, India*

Realizing maximum tumor suppression along with preventing tumor regrowth by optimizing the photons usage in phototherapy remains a major challenge. Herein, a mitochondrial-targeted phototheranostic nano-formulation (MsPDTT NPs) was prepared from molecular theranostic encapsulated into phospholipids. Notably, under single 690 nm laser excitation, MsPDTT NPs can perform dual-mode photoacoustic and near-infrared fluorescence (PA/NIRF) imaging and potent PDT/PTT due to efficient excited-state deactivation pathways (through radiative and energy transfer to generate reactive oxygen species and non-radiative relaxation). The reference RsPDTT NPs lacking mitochondrial targeting feature exhibits only PTT property. Based on biological results, MsPDTT NPs therapeutic response can be switched to PDT and PTT under a normoxic and hypoxic environment and maximize the overall efficacy of phototherapies without any noticeable side-effects. The current finding suggests the potential of using simultaneous PDT/PTT with proper photon utilization as a promising theranostic approach for hypoxic tumor photoablation.

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Poster Presentation : **ORGN.P-551**

Organic Chemistry

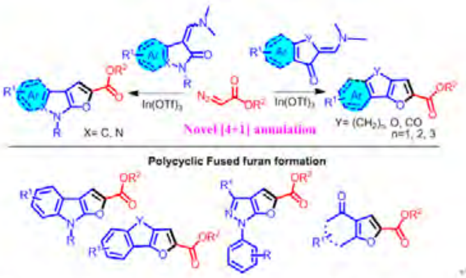
Event Hall FRI 11:00~13:00

Lewis-Acid Catalyzed Divergent-Orientated Regioselective Construction of Various Polycyclic Fused Furans

Jihwan Gim

School of Chemical Engineering, Yeungnam University, Korea

Furan is a crucial core moiety that is used as a versatile building block for the construction of a variety of functionalized molecules, present in many bioactive natural products, pharmaceuticals, and functional polymers. Diazo compounds are widely used for the synthesis of heterocycles in organic synthesis. Numerous transition metal-catalyzed transformations of diazo compounds have been well reported to effectively afford functionalized molecules. A variety of synthetic methods for fused furans have been reported included decarboxylative annulation of α,β-alkenyl carboxylic acids with cyclic ketones, ruthenium-catalyzed oxygenative [2+2+1] cycloaddition of silyldiynes with nitrones, and gold(I)-catalyzed intramolecular α-alkenylation of β-yne-furans. However, Lewis acid-catalyzed reactions have not been discussed in detail.Owing to the importance of diazo compounds and enaminones, herein we report the In(III)-catalyzed reactions of readily available β-enamino carbonyls with α-diazoacetates to afford divergently orientated polycyclic fused 2-carboalkoxyfurans (Scheme 1). This protocol also provides diversely functionalized polycyclic fused furans, which are formed in a significantly different manner to the reported 2-aminofurans in terms of the reaction pathway and product regiochemistry.



Scheme 1. Lewis acid-catalyzed synthesis of divergent-orientated fused 2-carboalkoxyfurans via [4+1] annulation

Poster Presentation : **ORGN.P-552**

Organic Chemistry

Event Hall FRI 11:00~13:00

Carbon nanotubes immobilized on gold electrode as an electrochemical humidity sensor

Jinhee Kim, Ueon Sang Shin[1,*]

Department of Nanobiomedical Science & BK21 PlUS NBM Global Research Center for Regenerative Medicine, Dankook University, Korea
[1]*Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Korea*

Multi-walled carbon nanotubes (MWCNTs) were fabricated on a gold electrode to develop a resistance-sensinghumidity sensor with low resistance. Core-shell-structured nanohybrids were prepared using Chitosan-MWCNTto obtain good hydrophilicity, resulting in a highly responsive humidity sensor. We also measured resistance,which changes due to hydrogen bonding between the amine group of chitosan and H2O. The structure of thefabricated chitosan-MWCNT core–shell-structured nanohybrid was measured. Furthermore, we determined thehighest response and linearity of the CS-MWCNT25 nanohybrids based on the number of coats on the electrodeand the composition ratio of chitosan and MWCNTs. The fabricated CS-MWCNT25 nanohybrid humidity sensorexhibited good electrical efficiency without voltage or frequency dependence and a low-temperature dependency with a temperature coefficient (RH/°C) of 0.187%. Finally, a fast recovery time of 40 s between 30%and 100% RH, a maximum humidity hysteresis of less than 0.300 ± 0.001%, and long-term stability for 2months indicated that this is an excellent humidity sensor.

Poster Presentation : **ORGN.P-553**

Organic Chemistry

Event Hall FRI 11:00~13:00

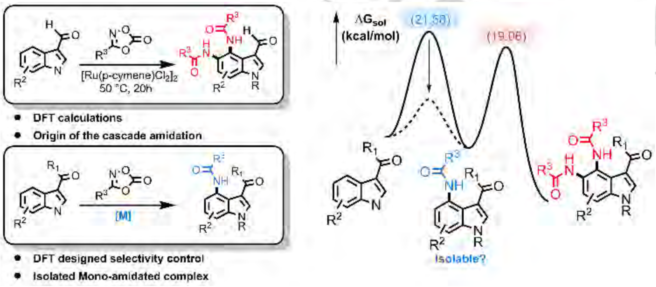
Transition Metal-Catalyzed Regio- and Chemo-selective Amidation of Indoles

Seok Yeol Yoo, Yong Rok Lee[1], Mu-Hyun Baik[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Division of Chemical Engineering, Yeungnam University, Korea*

Indole, aromatic N-heterocyclic compound, is one of the most important molecule in pharmaceuticals and natural products. Because of this importance, functionalizations of indoles, especially alkenylation and alkylation reactions have been widely studied. Despite the efforts, the amidation by utilizing dioxazolone is still elusive except the cobalt-catalyzed C2-amidation by Wang group.[1]Herein, we investigated the mechanism of direct ruthenium-catalyzed diamidation on C4- and C5- carbon of indole derivatives.[2] Density functional theory calculations were used to investigate the origin of selective diamidation. We have shown the detailed mechanism where the implemented amide enables the cascade C5-amidation. With the mechanism in hand, the chemo-selectivity control is on the investigation by metal and substrate tuning. The preliminary results shows the only mono-amidated product is observed without giving di-amidated product.



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Poster Presentation : **ORGN.P-554**

Organic Chemistry

Event Hall FRI 11:00~13:00

Formation of extremely thin pheomelanin-like film and its emergent properties

Seong Ah Jo, Kyungtae Kang[1,*]

Applied chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Since its discovery, polydopamine films have been intensively studied and applied to many materials fields, due to their material-independent deposition property and ease of further covalent functionalization. Although melanin pigments in nature, which are chemically similar to polydopamine, have multiple structural variations depending on where they are located and what their function is, polydopamine films have been seldom derivatized from the initially developed form. Inspired by natural pheomelanin—a cysteine-added derivative of eumelanin, we studied the deposition and physicochemical properties of polydopamine films synthesized with various cysteine derivatives as an additive. We found that addition of cysteine methyl ester or cysteine ethyl ester during polydopamine synthesis lead to the formation of an unprecedentedly thin (nearly monolayer-level) pheomelanin-like film with intriguing photo-responsive and electron-transferring properties. We showed the potential of this newly found pheomelanin-like particles as a bioinspired metal-free electrocatalyst for oxygen evolution reaction.

Poster Presentation : **ORGN.P-555**

Organic Chemistry

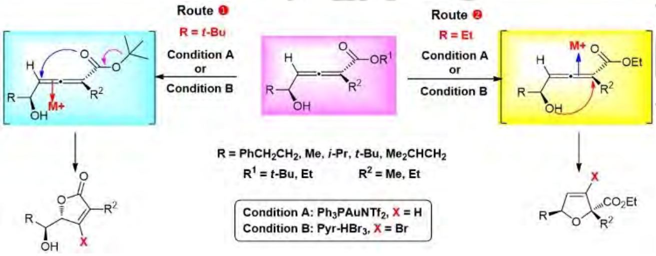
Event Hall FRI 11:00~13:00

Regiospecific Oxacyclizations of 5-Hydroxy-2,3-allenoates Via Gold Catalysis and Bromination

Zhang Aimin, Jisu Kim, Seungyeon Ryu, Jihye Lee, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

The availability of efficient synthetic methods in the construction of cyclic systems via organotransition metal catalysts is of considerable current interest in organic chemistry. In this regard, an allene has been proven to be a useful substrate for a variety of transition metal catalytic reactions, particularly for the cyclizations in the construction of carbo- and heterocycles. Recently, we disclosed new synthetic methods for the synthesis of 5-hydroxy-2,3-allenoates in regio- and stereospecific manner from the reaction of 1-alkyl allenoates and chiral bromoborane with aldehydes. As a part of an application, regiospecific cyclizations of 5-hydroxy-2,3-dienoates via gold catalysis (condition A) or bromination (condition B) were demonstrated to produce gamma-lactones (Route 1) or dihydrofurans (Route 2) in stereospecific manner. We will present scope and limitation of the oxacyclizations.



Poster Presentation : **ORGN.P-556**

Organic Chemistry

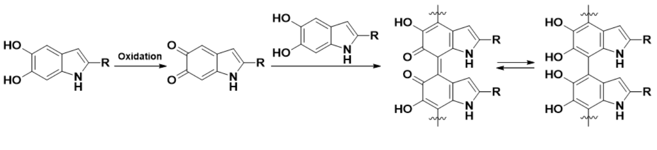
Event Hall FRI 11:00~13:00

Studies on the Electron Transfer Properties of Catechol System; Dihydroxyindole Derivatives under Visible-Light Irradiation.

Yuri Kim, Eun Joo Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Complex systems exhibit various emergent properties that appear macroscopically unpredictable by simultaneous interactions, which has the characteristic of reversibly controlling electron/energy systems. The most widely known complex system of catechol is melanin, of which eumelanin has a regular 5,6-dihydroxyindole(DHI) polymer backbone structure. However, due to their complex and systematically aggregated behavior, the precise chemical structure and function are not well known.[1] Pioneering works of Melchiorre and You group, which demonstrated direct alkylation of indole and intramolecular dearomatization of indole through electron donor-acceptor complex formation, showed the possibility of electron transfer properties through radical pathway of indole under visible-light.[2] Here, we began to explore to understand the biological function of the catechol complex system and DHI monomer by investigating their redox properties at the molecular level. Further study toward mechanistic elucidation are underway and these studies can develop new materials with optimized electron/energy transfer efficiency based on the catechol system, and various emergent property such as surface coating and radical properties are expected.



Poster Presentation : **ORGN.P-557**

Organic Chemistry

Event Hall FRI 11:00~13:00

Reactivity-Based FRET Probe for Imaging of Iron(II) Using Modification of non-Heme Enzyme

UHyeok Kim, Byungsun Jeon[1,*]

Center for Neuro-Medicine, Brain Science Institute, Korea
[1]*Korea Institute of Science and Technology, Korea*

Iron functions transport, storage and used of oxygen, electron transfer, DNA synthesis, metabolic reactions, ferroptosis and high redox activity. However, this same powerful redox abil-ity makes iron in undesirable forms harmful to the cell, because of its ability to promote oxidative stress by participating in processes like the Fenton reaction where iron catalyzed dis-proportionation of hydrogen peroxide can generate potentially toxic reactive oxy-gen species. Reactive oxygen stress caused various diseases including cardiovascular, neurodegenerative disorders, numerous cancers and aging. The reason why its function can be performed is that it occurs as Fe(II) and Fe(III) in their stable redox states. we desgin a novel reactivity-based FRET probe for imaging of Fe(II) using modification of non-Heme enzyme. We confirm the selectivity of this probe for fenton reaction in living system or changes to intracellular oxidation states. To use this strategy, we can notice change of labile iron pools in response to extracellular iron conditioning, overexpression of iron storage and/or export proteins, and post-translational downregulation of iron export by the peptide hormone hepcidin.Iron, one of the most abundant transition metal in Earth, is an essential element to pursue various functions in our body. Its redox activity between different oxidation states is required for the processes of oxygen transport, nucleoside synthesis, and epigenetic regulation. However, imbalance of its homeostasis, or misregulation of the iron makes it become a dangerous toxin that can trigger oxidative stress and cell damage. To monitor and sequester easily accessible iron in biological system, here, we design and synthesize a novel reaction-based FRET probe for Fe(II). The probe motivated by non-Heme enzyme catalysis exploits iron-mediated oxidative C-O bond cleavage to achieve diminished FRET phenomena. In this poster, we will describe our strategy how to design and synthesize the iron selective probe. In vitro and in vivo results will also be followed to validate its iron selectivity and reactivity.

Poster Presentation : **ORGN.P-558**

Organic Chemistry

Event Hall FRI 11:00~13:00

Indium(III)-catalyzed one-pot multicomponent N-annulation to polycyclic fused pyridines as potential optical chemosensors

Sana Jamshaid

Division of Chemical Engineering, Yeungnam University, Korea

Pyridines are utilized as building blocks for the construction of natural products, chiral ligands, complex molecules, pharmaceuticals, agrochemicals, and functionalized materials. They exhibit several biological and pharmaceutical activities and have been used as medicines to treat various diseases. Numerous synthetic strategies for pyridines have been developed, in contrast just a few synthetic approaches to fused pyridines bearing diverse polycycles have been demonstrated.Herein, we report a novel protocol for the construction of diversely fused pyridines containing tetracyclic rings by In(III)-catalyzed, solvent-free, one-pot N-annulation of enolizable ketones with N,N-dimethylformamide dimethyl acetal, ammonium acetate, and cyclic 1,3-dicarbonyl compounds through four-component reactions. In addition, we describe the formation of highly fused pyridines containing a pentacyclic ring via the reaction of two benzocycloalkanone molecules with N,N-dimethylformamide dimethyl acetal, and ammonium acetate (Scheme 1). These are novel and rapid syntheses of a variety of dihydrobenzoquinolines, azafluorenes, azafluorenones, pyridocoumarins, and benzocycloheptapyridines. The synthesized products were then evaluated for their potential use as optical chemosensors.

Scheme 1. An In(III)-catalyzed solvent-free multicomponent one-pot N-annulation for the construction of highly fused pyridines is developed as novel fluorophores.

Poster Presentation : **ORGN.P-559**

Organic Chemistry

Event Hall FRI 11:00~13:00

Effect of substituent on rate of reaction for detection of mercury and methyl mercury using a fluorescent probe bearing a boronic acid as a reactive site.

Sumita Subedi, Keun Hyeung Lee[1,*]

Department of chemistry, Inha University, Nepal

[1]*Department of Chemistry, Inha University, Korea*

Phenylboronic acids have been widely employed as important intermediates for various organic syntheses and reversible receptors for glucose and carbohydrates. We had already reported a new ratiometric fluorescent chemodosimeter for Hg2+ based on an irreversible reaction of phenylboronic acid with Hg2+. The fluorescent chemodosimeter (1) bearing a phenylboronic acid as a reaction site showed a selective and sensitive ratiometric signal behavior to low concentrations of Hg2+ ions in aqueous solution is containing 1% CH3CN. Even though, the selectivity and sensitivity of chemodosimeter (1) was very good but the rate of reaction was very slow. So in order to study of effect of electrondonating group in rate of reaction we introduce electrondonating methoxy group in phenylboronic acid. As expected the rate of reaction of displacement reaction increase compared to sensor without donating group. Electron donating group increases the electron density in aromatic ring of phenylboronic acid stabilizing the sigma complex which lowers the transition state energy and increases the rate of reaction. The fluorescence signal of mercury was not considerably inhibited by presence of other metal ions. The detection limit was measured to be 7.0 nM for Hg2+ based on the linear ratiometric signal to the nanomolar concentration (0–500 nM) of mercury ions. The signal mechanism study revealed that 1 reacted with Hg2+, providing covalent product of mercury ion (3) by replacement reaction of the boronic group of 1 with Hg2+, which exhibited fluorescent spectrum changes.

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Poster Presentation : **ORGN.P-560**
Organic Chemistry
Event Hall FRI 11:00~13:00

Detection of lead ions ratiometrically in aquatic environment and living cells using a fluorescent peptide-based probe

Mehta Pramod Kumar, Keun Hyeung Lee[1,*]

Department of Chemistry & Chemical Engineering , Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

Ratiometric fluorescent detection using dual emission bands is highly recommended to quantify Pb(II) in aquatic environment and live cells. We synthesized a ratiometric fluorescent peptidyl probe (1) by conjugation of a peptide receptor for Pb(II) with an excimer-forming benzothiazolylcyanovinylene fluorophore. Upon addition of Pb(II) (0-20 μM), the emission maximum shifted from 538 nm to 575 nm and the emission intensity ratio (I575/I538) increased significantly from 0.40 to 2.26. 1 exhibited a selective ratiometric response to Pb(II) over other metal ions. 1 with a low detection limit (1.2 ppb) of Pb(II) detected nanomolar concentrations (0-500 nM) of Pb(II) ions in groundwater and tap water. The cell-permeable probe detected intracellular Pb(II) by ratiometric fluorescent images. The binding mode study using 1HNMR, IR and CD spectroscopy, and TEM revealed that the probe formed a 1:1 complex with Pb(II) and then formed red-emissive nanoparticles and fibrils. The probe exhibited desirable detection properties such as ratiometric detection, high solubility in water, visible light excitation, high selectivity and sensitivity for Pb(II), cell-permeability, and rapid response (< 6 min).

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Poster Presentation : **ORGN.P-561**

Organic Chemistry

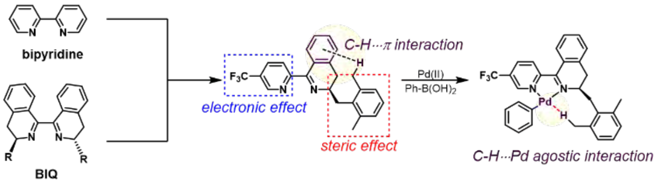
Event Hall FRI 11:00~13:00

Development of chiral Pyridine-Dihydroisoquinoline ligands for the Palladium-Catalyzed Addition of Arylboronic Acids to Alkenes: Insights from Computation and Experiment

Huijeong Ryu, **Sukwon Hong***

Department of Chemistry, Gwangju Institute of Science and Technology, Korea

In the last few decades, privileged chiral catalysts have achieved remarkable asymmetric synthesis. The new dihydroisoquinoline-based ligands developed by our group were aimed to generate a chiral environment that extended toward the metal center. Herein, we report the design, synthesis, and application of pyridine-dihydroisoquinoline(PyDHIQ) ligands, shown to be very efficient for addition of arylboronic acids to alkenes. In addition, the origin of reactivity and enantioselectivity in Pd-catalyzed 1,4-conjugate addition of 2-methyl chromones using PyDHIQ is explored using density functional theory computations. Benzyl group at the 2-position of the dihydroisoquinoline rings provides significant agostic interaction between it and palladium, thus stabilizing the activation energy in the transmetalation step to generate a phenyl-palladium complex and remarkably enhancing the reactivity. DFT calculations disclosed that the C-H•••π interaction between C-H bond of benzyl group and dihydroisoquinoline enables stable TS, resulting in high stereoselectivity. These results are expected to stimulate further application ㄴ of dihydroisoquinoline-based ligand as a useful chiral framework in enantioselective reactions.



Poster Presentation : **ORGN.P-562**

Organic Chemistry

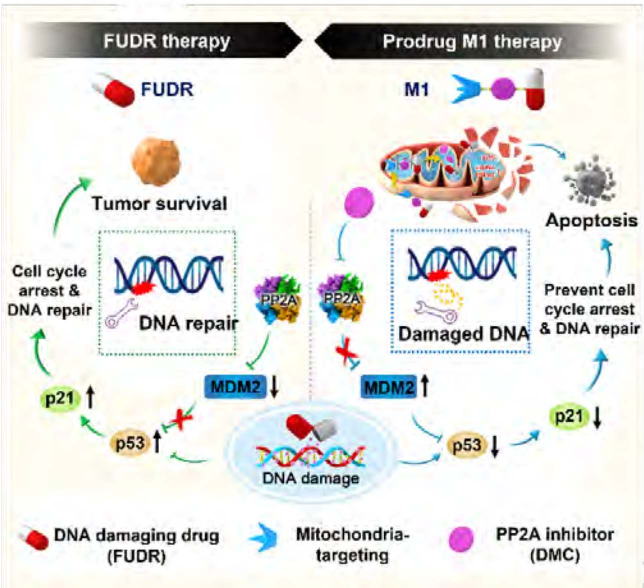
Event Hall FRI 11:00~13:00

DNA-Damage-Response-Targeting Mitochondria-Activated Multifunctional Prodrug Strategy for Self-defensive Tumor Therapy

Paramesh Jangili, Ji Hyeon Kim, Jusung An, Yuvin Noh, Ilwha Kim, Jongseung Kim*

Department of Chemistry, Korea University, Korea

The DNA damage response, which includes DNA repair and cell cycle checkpoint pathways originating from cancer cells, has been considered one of the main impediments to traditional chemotherapy and highlights the necessity to develop its targeting strategies. We develop a novel multifunctional construct, M1, designed explicitly to target the DNA damage response in cancer cells. M1 contains both a floxuridine (FUDR) and protein phosphatase 2A (PP2A) inhibitor combined with a GSH-sensitive linker. Further conjugation of the triphenylphosphonium moiety allows M1 to undergo specific activation in the mitochondria, where mitochondria-mediated apoptosis is observed. Moreover, M1 has enormous effects on genomic DNA ascribed to FUDR's primary function of impeding DNA/RNA synthesis combined with diminishing PP2A-activated DNA repair pathways. Importantly, mechanistic studies highlight the PP2A obtrusion in FUDR/5-fluorouracil (5-FU) therapy and underscore the importance of its inhibition to harbor therapeutic potential. HCT116 cell xenograft-bearing mice that have a low response rate to 5-FU show a prominent effect with M1, emphasizing the importance of DNA damage response targeting strategies using tumor-specific microenvironment-activatable systems.


FUDR therapy
Prodrug M1 therapy
FUDR
M1
Tumor survival
Apoptosis
Cell cycle arrest & DNA repair
DNA repair
PP2A
PP2A
Damaged DNA
Prevent cell cycle arrest & DNA repair
MDM2 ↓
MDM2 ↑
p21 ↑
p53 ↑
DNA damage
p53 ↓
p21 ↓
DNA damaging drug (FUDR)
Mitochondria-targeting
PP2A inhibitor (DMC)

Poster Presentation : **ORGN.P-563**
Organic Chemistry
Event Hall FRI 11:00~13:00

Cyrene™ as a Neoteric Bio-based Solvent for Catalyst-free Microwave-Assisted Construction of Bipyridine Scaffolds for Heavy-Metal Sensing

Peter Yuosef Rubio

School of Chemical Engineering, Yeungnam University, Korea

Sustainable synthesis has attracted significant attention from researchers in various fields. Eliminating the use of traditional, dangerous solvents while promoting the use of viable and safe alternatives has become a top priority. Recently, dihydrolevoglucosenone (Cyrene™) has received significant attention as a neoteric green, economically sustainable and environmentally benign solvent from residual biomass. Cyrene™ is used as a solvent in many processes, including SNAr and SN2 reactions, Pd-catalyzed coupling, nucleophilic addition, MOF synthesis, and graphene production. Furthermore, its excellent water compatibility and elevated boiling point make it suitable for use in various organic syntheses. In this work, we employed the use of insufficiently basic amine substrates, additive- and catalyst-free microwave condition compatible with Cyrene™ solvent.This environment-friendly synthetic protocol was developed to access polyfunctionalized bipyridines from readily available amines, chromone-3-carboxaldehydes, and pyridinylacetonitriles under catalyst- and additive-free conditions using bio-renewable neoteric solvent dihydrolevoglucosenone (Cyrene™). In this strategy, amines serve as both a mild-base promoter and a substrate. In addition, water is the only by-product of this reaction. This multi-component protocol provides highly diverse 2,3-, 3,3-, and 3,4-bipyridines in good-to-excellent yields. Operational simplicity, short reaction time, excellent atom economy, and easily obtainable substrates are among the features of this microwave-assisted synthesis. Additionally, the compounds synthesized via this method have demonstrated the ability to detect heavy metals, specifically mercury(II), copper(II), and iron (III) ions.

Scheme 1. Catalyst- and additive-free strategy for the formation of 2,3'-bipyridine analogues.

Poster Presentation : **ORGN.P-564**

Organic Chemistry

Event Hall FRI 11:00~13:00

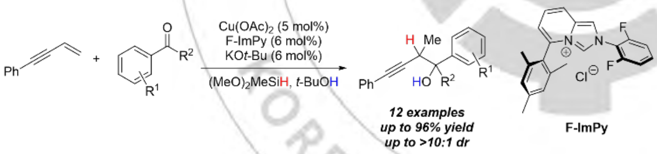
Fluorinated N-Heterocyclic Carbene Ligands for Cu-Catalyzed Diastereoselective Addition Reactions

Woosong Han, Sukwon Hong[1,*]

Chemistry, Gwangju Institute of Science and Technology, Korea

[1]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

Imidazo[1,5-a]pyridine-3-ylidene carbene ligand (ImPy) derivatives derived in two steps from readily available 6-mesitylpicolinaldehyde were developed. The ImPy-Cu complex was characterized by NMR, X-ray crystallography and is an effective catalyst for the diastereoselective addition of 1,3-enyne nucleophile to ketones showing good yields (up to 96%) high diastereoselectivities (up to >10:1).



Poster Presentation : **ORGN.P-565**

Organic Chemistry

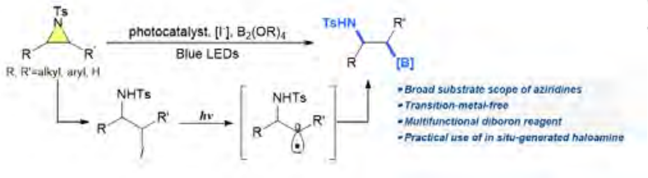
Event Hall FRI 11:00~13:00

A tandem process for the synthesis of β-aminoboronic acids from aziridines with haloamine intermediates

Subin Park, Hong Geun Lee[1,*]

Department of chemistry, Seoul National University, Korea
[1]*Department of Chemistry, Seoul National University, Korea*

Herein, we have developed a novel strategy for the synthesis of β-aminoboronic acids. The aziridine ring-opening reaction by using nucleophilic iodide sets off a cascade process, in which an in situ-generated haloamine intermediate serves as a precursor for subsequent radical borylation. The developed protocol enabled the preparation of β-aminoboronic acids from various types of substrates that were not suitable for previous approaches. Eventually, the method has successfully expanded the synthetic utility of aziridines compared to previous methods. During our investigation, an unexpected participation of diboron reagent in the aziridine opening step was identified, which critically facilitated the overall transformation. The finding will eventually contribute to drug design processes that are based on β-aminoboronic acids, a pharmaceutically important motif.



Poster Presentation : **ORGN.P-566**

Organic Chemistry

Event Hall FRI 11:00~13:00

High intensity focused ultrasound-responsive Microbubble Drug Delivery for the Treatment of Malignant Glioma

Been Yoon, Myoung-Hwan Park[1,*]

Convergence science, Sahmyook University, Korea
[1]*Department of Chemistry, Sahmyook University, Korea*

Malignant gliomas are composed of two small cell populations characterized by proliferation and migration. Cell invasion and proliferation of glioma cells are mutually exclusive. Proliferating cells have less migration and proliferate quickly on the spot, but migrating cells have the property of slowly dividing. Therefore, surgical treatment, radiation therapy, and chemotherapy are performed according to the characteristics of the cells. Chemotherapy has a limited number of drugs that cross the BBB (Blood-Brain Barrier) If it recurs, there is the problem of resistance to existing drugs. To overcome the limitations of BBB opening and limited drug use, this study uses High intensity focused ultrasound (HIFU) for BBB opening and patient-specific drug-surfaced microbubble. Microbubble are composed of shell and gas, the shell binds the drug to the ester bond to the synthetic lipid, and the gas uses PFPs. This mechanism uses ultrasonic waves (1W, 1MHz, 5% DC, 120s) to break microbubble and locally release high temperature and high pressure, which breaks down the ester bond and releases the drug. The analytical method in this study confirmed the synthesis and hydrolysis of drug carrier by NMR. The concentration of the bubble and the drug attached to the bubble were confirmed by OM(Optical Microscopy) and Confocal Microscopy. Confirmed by ultrasound The drug release test was analyzed by HPLC. We are proceeding with in vitro experiments using U87MG cells, selecting mouse as an animal model, and conducting in vivo experiments. Treatment of brain tumors is still difficult. This study has the advantage that various drugs can be introduced according to the patient, and It will make a great contribution to the treatment of brain tumors in the future.

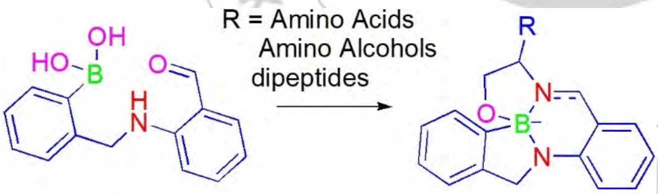
Poster Presentation : **ORGN.P-567**
Organic Chemistry
Event Hall FRI 11:00~13:00

Photogeneration and Quenching of Reactive Oxygen Species by boronic acid aldehyde Probe

Mukesh Shirbhate, Kwan Mook Kim[1,*]

Chemistry, Ewha Womans University, Korea
[1]*Department of Chemistry, Ewha Womans University, Korea*

A new paradigm bio-orthogonal click-reaction probe that photosensitizes a specific protein to prevent cancer cells and viruses/resistant bacteria to be applied to diagnosis and treatment. In particular, human serum albumin (HSA) is concentrated in cancer tissues. The main goal is to develop a photodynamic cancer treatment agent by applying the appropriate properties. In this connection, we design and synthesize new Click Probes such as 1, and 2 (figure 1) bind amino acids, dipeptides, tripeptides, etc. can create an interesting fluorescent and CD.



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Poster Presentation : **ORGN.P-568**

Organic Chemistry

Event Hall FRI 11:00~13:00

N-iodosuccinimide (NIS) Mediated Transformations of Benzylic C(sp^3)–B Bond to Various C(sp^3)–Heteroatom Bond

JuHyun Youn, Hong Geun Lee[*]

Department of Chemistry, Seoul National University, Korea

Here in, we demonstrate the transformation of benzylic C(sp^3)–B bond to C(sp^3)–heteroatom bond by N-iodosuccinimide (NIS) facilitation. Various heteroatom nucleophiles can be introduced with high tolerance of functional groups under mild reaction conditions. Mechanistic studies suggested that the reaction could proceed with the corresponding iodide species as the reaction intermediate which is activated by halogen bonding with NIS.

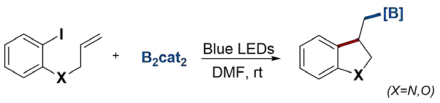
Poster Presentation : **ORGN.P-569**
Organic Chemistry
Event Hall FRI 11:00~13:00

Catalyst-free photoinduced 1,2-arylboration via Csp2–I activation for the synthesis of heterocycle

Jihye Kang, Hong Geun Lee*

Department of Chemistry, Seoul National University, Korea

A green and sustainable method for the synthesis of heterocycle has been developed; a catalyst-free 1,2-arylboration using only blue LED light. Heterocyclic compounds are important and prevalent structural motifs in biologically active molecules and drugs. Therefore, there is a continuing interest in the development of protocols for the synthesis of indolines and 2,3-dihydrobenzofuran scaffolds. Moreover, borylated heterocyclic compound has many potential advantages of being transformed into various useful functional groups which could maximize structure diversity. We focused on multiple bond forming transformations, including multicomponent reactions, which make possible to synthesize target molecules with greater efficiency and atom economy. This sequential strategy would allow access to the simultaneous formation of two different bonds such as C–X or C–B with one C–C bond, which is known as “carbofucnctionalization”. Along these lines, we envisioned that carboboration strategy would establish C–B bond to the heterocyclic compound. Several carboboration method using transition metal have been already reported. However, there is limitted carboboration method which involves radical cascade strategy. Our newly developed transition metal free approach could serve as a de novo protocol to access diversely substituted indoline and dihydrobenzofuran derivatives under mild conditions. Not only intramolecular reaction, intermolecular arylboration is also found to be compatible with this reaction condition. Further functionalization was enabled based on the versatility of boron substituted compound.



- *Metal and additive-free*
- *1,2-carboboration*
- *Redox neutral*
- *Synthesis of Heterocycle*

Poster Presentation : **ORGN.P-570**

Organic Chemistry

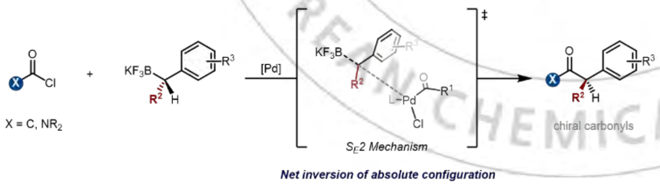
Event Hall FRI 11:00~13:00

Stereospecific Acylative Suzuki-Miyaura Cross-Coupling: Synthesis of Optically Active α-Aryl Carbonyl Compounds

Byeongdo Roh, Hong Geun Lee*

Department of Chemistry, Seoul National University, Korea

Disclosed is the first stereospecific acylative Suzuki–Miyaura cross-coupling reaction of enantiomerically enriched acyclic secondary alkylboron compounds. The reaction is achieved with complete inversion of stereochemistry, providing access to optically active ketones and amides bearing stereogenic tertiary carbon center at alpha-position. The resulting stereochemistry is rarely dependent of any electronic and steric properties of both ligands and substrates. On the basis of further computational studies, it is suggested that the reaction proceeds with transmetalation step via open SE2 mechanism which backside attack of the palladium complex on the benzylic carbon atom of alkyl trifluoroborates occurs, resulting in exclusive inversion of stereochemistry.



Poster Presentation : **ORGN.P-571**

Organic Chemistry

Event Hall FRI 11:00~13:00

The study of chemical reaction process for decomposing 2-Chlorobenzalmalononitrile(CS) , known as a major component of chemical weapon named tear gas.

Youjin Mun, Kwan Mook Kim[1,*]

Nano chemistry bio chiral lab, Ewha Womans University, Korea

[1]*Department of Chemistry, Ewha Womans University, Korea*

2-Chlorobenzalmalononitrile, which is generally known as a tear gas or CS gas, is a chemical weapon which stimulates the nerves of the lacrimal gland in the eye to produce tears. This chemical weapon is usually used by law-enforcement agencies in many countries to control mobs or rioters. The CS gas is not itself a gas phase, but a powder form and can be dispersed in the air through use of sprays, fog generators, grenades. When It is dispersed in the air, its residue settles on surfaces and stays there for days before break down. Therefore, here we studied the decomposing process of CS gas, using an alkaline solution with an adequate conditions to accelerate the decomposing process of CS gas, producing 2-Chlorobenzaldehyde and Malononitrile.

Poster Presentation : **ORGN.P-572**

Organic Chemistry

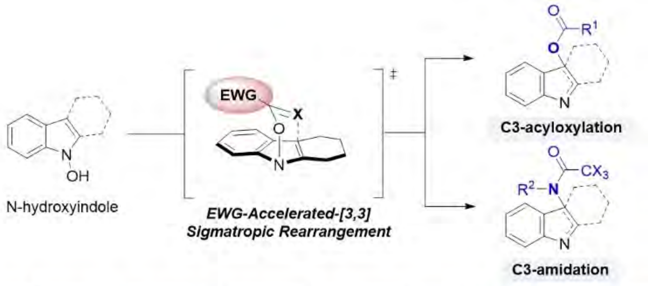
Event Hall FRI 11:00~13:00

C3-Hetero-functionalization of Indole Derivatives Enabled by [3,3]-Sigmatropic Rearrangement Activated by Electron-Withdrawing Group

Yujin Lee, Hong Geun Lee*

Department of Chemistry, Seoul National University, Korea

A novel C3 hetero-functionalization method for indoles via EWG-accelerated-[3,3] sigmatropic rearrangement of N-hydroxyindole has been developed. The reaction exhibited high efficiency under mild conditions, and was therefore applicable to the preparation of a wide range of indole derivatives including 3-aminoindoles, 3-aminopyrrolindoline and 3-aminoindolenines. This reaction relies upon the activation of C=N double bond by electron-deficient trichloromethyl group, and proceeds with the high practicality and scalability. Based on mechanistic investigations, the reaction proceeds via the conventional concerted [3,3] mechanism as a major pathway, however, dissociation-recombination mechanism also takes part as a minor pathway. The underlying intrinsic reason of exceptional acceleration phenomenon from EWG group is under investigation.



- ♦ Electronically designed [3,3] sigmatropic rearrangment applied in C3-functionalization
- ♦ Simple, easy set-up ♦ Mild reaction condition

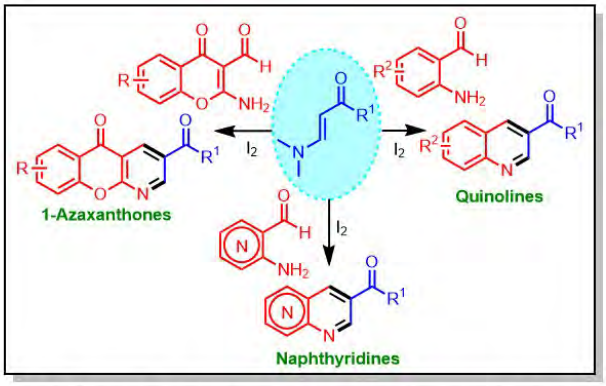
Poster Presentation : **ORGN.P-573**
Organic Chemistry
Event Hall FRI 11:00~13:00

Iodine-Catalyzed Annulation Approach to Diverse N-Heteroctycles

Hari Datta Khanal

School of Chemical Engineering, Yeungnam University, Korea

Nitrogen-containing heteroaromatics are present in natural and synthetic products, as well as in pharmaceuticals. Among them, azaxanthone, quinoline, and naphthyridine derivatives share the basic pyridine-ring framework and are important scaffolds in many natural and synthetic materials that exhibit broad pharmacological properties, including analgesic, antiarthitic, anti-inflammatory, antitumor, and HIV-inhibitory activities.Owing to their utility and applications, a variety of methods for the syntheses of azaxanthone, quinoline, and naphthyridine derivatives have been reported. Traditional synthetic routes to quinolines and naphthyridines include the Friedländer reaction of 2-aminobenzaldehyde with a carbonyl compound in an acidic or basic medium. However, the method is limited by regioselectivity problems when unsymmetrical ketones are used. Azaxanthones have been prepared by the reactions of 2-chloronicotinic acid with substituted phenols followed by cyclization under basic conditions in a three-step process. Despite the achievements for the construction of these N-heterocycles, more environmentally benign and facile protocols are highly desirable to minimize the use of toxic and expensive catalysts, harsh reaction conditions, and multi-step procedures.As a part of our ongoing study for the development of new methodologies for the synthesis of N-heterocycles under metal-free conditions, herein, we report an operationally simple one-pot heterocyclization method for the syntheses of 1-azaxanthones, quinolines, and naphthyridines that involves the mild I2-catalyzed annulations of 2-amino-3-formylchromones, 2-aminobenzaldehydes, and aminonicotinaldehydes with β-enamino esters and β-enaminones (Scheme 1).



Scheme 1. Our synthetic strategies to 1-azaxanthones, quinolines, and naphthyridines.

Poster Presentation : **ORGN.P-574**

Organic Chemistry

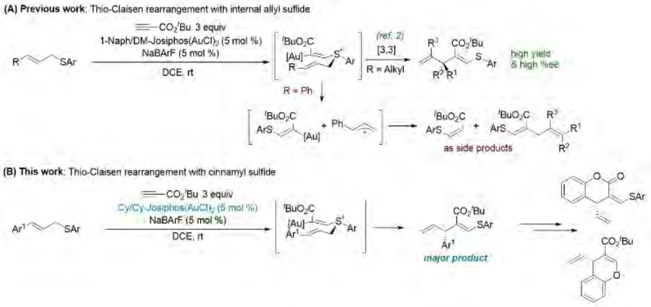
Event Hall FRI 11:00~13:00

Enantioselective Intemolecular Thioallylation of Cinnamyl Thioethers via Claisen rearrangemnet

Jiwon Jang, Youngjin Bae, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Formation of –onium salts is useful strategy to accelerate sigmatropic rearrangement. Recently, we reported an asymmetric Claisen rearrangement of sulfonium salts formed in-situ from the gold-catalyzed addition of thioethers to propiolates (Scheme 1A). Although high enantioselectivities were achieved with wide range of allyl groups, one disadvantage became apparent. Substrates having an aryl group as the terminal allyl substituent failed and generated only byproducts from the cleavage and a formal [1,3]-rearrangement. Through the extensive screening of ligands, we found that Cy/Cy-Josiphos ligand gave good product selectivity with exceptional enantiocontrol (Scheme 1B). A range of aryl group were tolerated at Ar^1 and some of the products could be transformed into a biologically active compounds having coumarin or chromene core that may have significant biological activity.



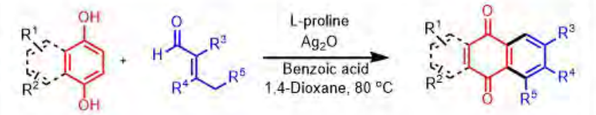
Poster Presentation : **ORGN.P-575**
Organic Chemistry
Event Hall FRI 11:00~13:00

Regioselective Construction of Diverse Quinone Derivatives via Benzannulation by Organic-Inorganic Dual Catalysis

Muhammad Saeed Akhtar

School of Chemical Engineering, Yeungnam University, Korea

Naphthoquinone derivatives are widely distributed in nature and are commonly used as pharmaceutical agents. These derivatives have been the focus of research efforts due to their diverse biological activities. The anthraquinone motif is also commonly found in natural products and incorporated into potential therapeutics and has been shown to confer diverse biological properties. In addition, the anthraquinone motif has been used to produce dyes, ligands, lead compounds, and drug candidates. Recently anthraquinone-based molecules have attracted research attention in the molecular electronics field.Due to their diverse applications and uses, many synthetic protocols have been developed to produce naphthoquinones and anthraquinones. Typical methods used to synthesize 1,4-naphthoquinones include the Diels-Alder reaction between quinones and 1,3-dienes and subsequent oxidation, NHC-catalyzed Stetter reaction, and palladium-catalyzed direct cross-coupling of 1,4-benzoquinones and vinyl ethers. Although several synthetic protocols have been reported for 1,4-naphthoquinones and anthraquinones, simpler, atom economic, and more effective methods are required. To date, no report has been issued on the synthesis of 1,4-naphthoquinone and anthraquinone derivatives by benzannulation of α,β-unsaturated aldehydes using substituted hydroquinones or naphthalene-1,4-diols. Here, we report a facile method for the regioselective construction of diverse 1,4-naphthoquinones and anthraquinones using silver- and secondary amine-catalyzed benzannulation of various α,β-unsaturated aldehydes and 1,4-benzenediols, or 1,4-naphthalenediols via domino quinone construction followed by formal [4+2] cycloaddition and oxidation (Scheme 1).



Scheme 1 Synthetic strategy for the construction of 1,4-naphthoquinones and anthraquinones from 1,4-benzenediols and 1,4-naphthalenediols.

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Poster Presentation : **ORGN.P-576**

Organic Chemistry

Event Hall FRI 11:00~13:00

Photochromic reaction of spiropyran derivatives with benzothiazole moiety

Go Eun Choi, Eun Ju Shin*

Department of Chemistry, Sunchon National University, Korea

Metals are found everywhere. Transition metals and heavy metals play an important role in biological, environmental, material, and industrial fields. Metal cation driven photochromic transformation of spiropyran has been incredibly widely used for detecting various metals based on colorimetry and fluorometry. Spiropyran undergoes isomerization between colorless nonfluorescent spiropyran and colored fluorescent merocyanine, upon external stimuli such as light, heat, pH, and metal cations. Therefore, a variety of spiropyran derivatives has been extensively studied since first discovery in the early 20th century and its photochromism discovered in 1952, due to their versatile application in diverse fields. However, there are few studies on benzothiazole derivatives. In this study, novel spiropyran derivatives with benzothiazole moiety were synthesized and characterized. It is interesting to investigate how the presence or absence of sulfur affects the spectral and photochromic properties of spiropyran derivatives. The absorption and fluorescence spectra of spiropyran derivatives with benzothiazole moiety were investigated with or without UV irradiation.

Poster Presentation : **ORGN.P-577**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fluorogenic detection of α-amylase activity in human urine using amphiphilic pyrene/γ-cyclodextrin inclusion complexes

Taemin Park, Anh.T.N Nguyen, Jun Ho Shim*, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

We have developed an effective fluorescent biosensor for sensitive detection of α-amylase activity on the basis of inclusion complexes between amphiphilic pyrenyl derivatives and γ-cyclodextrins (γ-CDs). The amphiphilic pyrenyl derivatives display the self-assembled nanofibrils in aqueous media, providing the hydrophobic π-extended conjugated system at the inner part and hydrophilic functionality at the periphery. Their monomer component is captured by γ-CD and degrades nanofibrils to form a dimer of the Py-CO2:γ-CD complex, which exhibits strong excimer fluorescence. Finally, nanofibrils are regenerated as γ-CD is degraded by α-amylase, with the result that excimer fluorescence decreases and monomeric fluorescence increases again. These structural changes drive highly selective and sensitive detection of α-amylase at very low concentrations by ratiometric fluorescence color changes.

Poster Presentation : **ORGN.P-578**

Organic Chemistry

Event Hall FRI 11:00~13:00

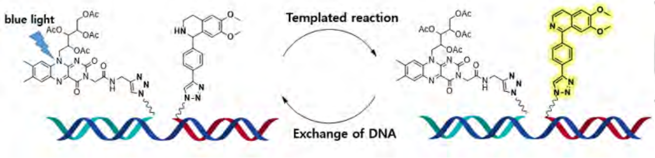
Riboflavin-Catalyzed Fluorogenic Photooxidation for Nucleic Acid Sensing

Hokyung Kim, Ki Tae Kim[1,*]

Chemistry, Chungbuk Natioanl University, Korea

[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

DNA-templated reactions proceed by high effective concentrations induced by hybridization of reactive oligonucleotides to a DNA template. The templated reaction is currently considered a powerful technology for nucleic acid detection due to signal amplification effects based on repeated cycles of a strand exchange and a chemical reaction. However, it is struggling with low reaction rates and signal amplification. To overcome such limitations, here, we report novel DNA-templated reactions based on riboflavin-catalyzed fluorogenic oxidation of a cyclic amine and a reduced rhodamine. The cyclic amine and reduced rhodamine are oxidized by riboflavin under blue-light irradiation to produce fluorescent signals. Using these new simple photoreactions, we effectively detect specific target nucleic acids with strong fluorescence signals.



Poster Presentation : **ORGN.P-579**

Organic Chemistry

Event Hall FRI 11:00~13:00

Two-Photon Fluorescence Probe for Imaging Cell Membrane Organization

Tanmay kumar Pati, Hwan Myung Kim[1,*]

ENERGY SYSTEM, Ajou University, Korea

[1]*Department of Energy Systems Research, Ajou University, Korea*

The important organelles of cell such as mitochondrion, ribosome, Golgi, lysosome, endoplasmic reticulum, and nucleus are protected from surrounding environment by cell plasma membrane. Cell plasma membrane plays important roles in cellular communication and signalling associated with different physiological and pathological processes. Fluorescence analysis is one of the suitable methods to understand the membrane related complex biological process. Utilization of environment sensitive turn on probe for visualization of membrane organism is superior alternative over the fluorescent labelling of lipids as labelling may alter its properties. On the other hand, development of bright two photon fluorescence probe is highly desirable because of its deep penetration, less photobleaching and superior spatial selectivity. Here we aim to design and synthesize a two photon probe that combines specific membrane targeting, on/off switching, and environment sensing functions.

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Poster Presentation : **ORGN.P-580**

Organic Chemistry

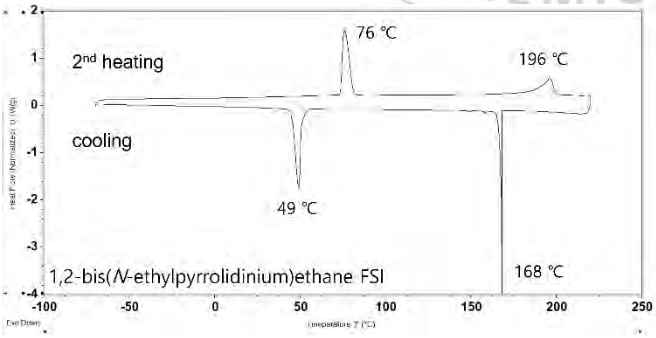
Event Hall FRI 11:00~13:00

Synthesis and characterization of 1,2-bis(*N*-alkylpyrrolidinium)ethane bis(fluorosulfonyl)imide

Seunghwan Kim, Minjae Lee[1,*]

Department of chemistry, Kunsan National University, Korea
[1]*Department of Chemistry, Kunsan National University, Korea*

Organic ionic plastic crystals (OIPCs) are a new class of solid electrolytes with significant advantages over conventional solid ion conductors because of their plasticity, non-flammability and high ionic conductivity. Our research group has explored new OIPCs including dicationic organic structures. As an anioin, Br^-, I^-, PF_6^-, TF_2N^-, and BF_4^- were studied with combination of the dications. In this study, bis(fluorosulonyl)imide (FSI) anion was applied to the bis-pyrrolidinium cations and the new compounds were characterized in detail. A series of 1,2-bis(*N*-alkylpyrrolidinium)ethane FSI salts were synthesized and their chemical structures were confirmed by ^{1}H NMR and FT-IR. Using differential scanning calorimetry (DSC), 1,2-bis(*N*-ethylpyrrolidinium)ethane FSI exhibited one solid-solid phase transition at T_{ss} = 76 ℃. This compound showed low entropy of fusion, 16 J $K^{-1}mol^{-1}$, which satisfies the Timmermans' definition of plastic crystals ($\Delta S_f < 20$ J $K^{-1}mol^{-1}$).



Poster Presentation : **ORGN.P-581**

Organic Chemistry

Event Hall FRI 11:00~13:00

Two-photon fluorescent probes based on pyrene for biomedical applications

Vinayak Juvekar, Hwan Myung Kim[1,*]

Department of Chemistry, Ajou University, Korea

[1]*Department of Energy Systems Research, Ajou University, Korea*

Development of fluorescent probes for two-photon microscopy is a beneficial in the biological application because of impressive light penetration depth and superior spatio selectivity. Herein we designed and synthesised organic fluorescent probe containing pyrene core for biological applications using two-photon microscopy. Developed probes showed marked two-photon absorption ability, impressive reactive oxygen species generation ability as well as fast loading ability into the cells and negligible dark toxicity. Live cell analyses with one and two-photon microscopy showed bright fluorescent images and photo-toxicity. These results indicates the developed two-photon probes could be useful in utilizing various biological applications and further designing various two-photon probes.

Poster Presentation : **ORGN.P-582**

Organic Chemistry

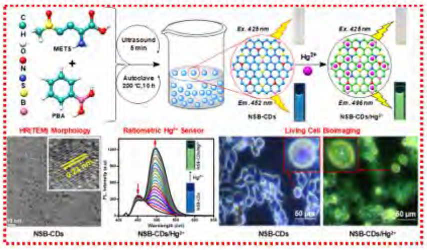
Event Hall FRI 11:00~13:00

Selective and sensitive ratiometric detection of Hg2+ ions in cell imaging based on photoluminescent carbon dots

Mohandoss Sonaimuthu

Department of Chemical Engineering, Yeungnam University, Korea

Mercury (Hg2+) can accumulate through the food chain and finally enter the human body. Hg2+can cause irreparable damage to kidney, nervous system and other organ systems. Therefore, there is an urgent need for a new probe for sensitive and selective ratiometric Hg2+ detection in aqueous solutions in the environment and living systems. Carbon dots (CDs) are significant figures in the field of nano-range fluorescent probes and considerable interest owing to their excellent water solubility, low cytotoxicity, ease of preparation, and environmental friendliness. Doping of carbon dots (CDs) with heteroatoms such as nitrogen (N), sulfur (S), phosphorous (P), boron (B), and fluorine (F) has become a popular way to tailor surface defects, tune the properties, and analyze new and interesting phenomena for sensing and live cell imaging applications.Inspired by these efforts, herein we report the synthesis of NSB-CDs with methionine sulfoxide and phenylboronic acid through a one-step hydrothermal method and its applications in ratiometric detection of Hg2+ using multicolor cell imaging is described (Scheme 1). The prepared NSB-CDs possess good aqueous solubility, excellent pH and ionic stability, excitation dependent, and high quantum yield. The NSB-CDs sensor exhibit high selectivity and sensitivity towards Hg2+ ions over other metal ions. The live cell of HCT-116 cells with NSB-CDs validates the application of multicolor imaging for the detection of Hg2+ ions in aqueous media and biological systems.



Scheme 1. The preparation of multiple heteroatom-doped photoluminescent carbon dots and its applications in ratiometric detection of Hg^{2+} using multicolor cell imaging.

Poster Presentation : **ORGN.P-583**

Organic Chemistry

Event Hall FRI 11:00~13:00

Dipolar small molecule dyes for two-photon photodynamic therapy

DongJoon Lee, **Hwan Myung Kim**[1,*]

Ajou University, Korea

[1]*Department of Energy Systems Research, Ajou University, Korea*

Photodynamic therapy (PDT) using two-photon process is a promising approach for the treatment of cancer because of its better penetration depth and superior spatial selectivity. Here, we describe chalcogen-containing small molecule dyes as a two-photon activated, type I based photosensitizer (PS). These dyes derived from an amine substituted naphthalene as an electron donor and electron acceptor such as benzimidazole (BN), benzoxazole (BO), and benzthiazole (BS). Among them, heavier chalcogens containing dyes showed marked reactive oxygen species (ROS)-generating ability under physiological conditions, as well as fast loading ability into the cells and negligible dark toxicity. Live cell and cancer tissue analyses with two-photon microscopy revealed that the PSs have effective PDT properties under 770 nm two-photon irradiation. The developed two-photon PS could be useful in efficient PDT applications and in designing various PSs.

Poster Presentation : **ORGN.P-584**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fluorination of 2-amidobenzo[b]thiophenes using N-Fulorobenzenesulfonimide

Won seok Choi, **Hyun-Suk Yeom[1,*]**, **SuJeong Hong[2]**, **So Yeun Lim[2]**

Chemistry, Hanyang University, Korea

[1]*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

[2]*Korea Research Institute of Chemical Technology, Korea*

Fluorine occupies a notable position, especially in the design of drug and agrochemical molecules due to its wideranging biological activities. Installation of fluorine into organic molecules provides unique opportunities to improve the metabolic stability. Modulation of lipophilicity can also be effectively done by selective incorporation of fluorine. Therefore, tremendous efforts have been devoted for development of strategies for C−F bond formation using various nucleophilic, electrophilic, and radical fluorinating agents such as tetrabutylammoniumfluoride (TBAF), N-fluoropyridinium triflate, XeF2, Selectfluor, N-fluorobenzenesulfonimide (NFSI) etc. Among the fluorinating agents, NFSI has attracted much interest because it is a nonhygroscopic, stable crystalline solid that is easy to handle and commercially available. Benzo[b]thiophenes are core structure having various biological activities such as antifungal agents, anti-inflammatory agents, estrogen receptor modulators, leukotriene formation inhibitor by 5-lipooxygenases inhibition. It also has the preventing effect against hepatitis C virus and malaria. Therefore, there have been longstanding interests for the synthesis and functionalization of benzo[b]thiophene. However, there are few reports on the fluorination of benzo[b]thiophene, so the development of an efficient fluorination method is of great significance. In this presentation, taking into consideration of the importance of both benzo[b]thiophene moiety and fluorine, we report a C-3 fluorination of 2-amidobenzo[b]thiophene under metal-free conditions

Poster Presentation : **ORGN.P-585**

Organic Chemistry

Event Hall FRI 11:00~13:00

Highly Sensitive Lipid Droplet Probe for In Vivo Two-Photon Imaging of Drug-Induced Liver Injury

Hyo Won Lee, Eun Seo Kim, Hwan Myung Kim*

Department of Energy Systems Research, Ajou University, Korea

Lipid droplets (LD) are lipid-rich organelles found in most cell lines and are mainly composed of neutral lipids. LDs are prominent in various diseases related to lipid control, such as obesity, fatty liver disease, diabetes, and arteriosclerosis. For monitoring LD dynamics in live samples, we developed a highly selective two-photon fluorescence tracker for LDs (LD1). It showed excellent sensitivity with a remarkable two-photon action cross-section (>600 GM), photostability, and cell loading ability. In human hepatocytes and in vivo mouse liver tissue imaging, LD1 showed bright fluorescence with high LD selectivity and minimized background signal to evaluate the nonalcoholic fatty liver disease (NAFLD) stages. Interestingly, we proved that the liver sinusoid morphology became narrower with growing LD size and visualized the moment including fusion of the LDs in vivo. In addition, real-time and dual-color TPM imaging using LD1 and a two-photon lysosome tracker could be a helpful predictive screening method in the drug development process to monitor impending drug-induced liver injury-inducing drug candidates.

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Poster Presentation : **ORGN.P-586**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of homoallylic amides through hydroamidation of allenes with DIBAL-H and isocyanates

Kyeongmin Lee, Yunmi Lee[1,*]

Chemistry, Kwangwoon University, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*

Amides are common and important functional groups existed in a variety of natural products, biologically active molecules and pharmaceuticals. Due to the significance of synthetic utility, various methods have been developed for the synthesis of amides. Conventional methods for the synthesis of amides are coupling reactions of activated carboxylic acid derivatives with amines using coupling reagents. In this presentation, we describe a new approach to amides starting from allenes and isocyanates. Hydroalumination of allenes with readily available diisobutylaluminum hydride was promoted by an N-heterocyclic carbene-based copper catalyst to generate allylic aluminum reagents in situ, which subsequently were reacted with isocyanates. This one-pot hydroamidation of allenes with isocyanate provided a variety of homoallylic amides bearing all-carbon quaternary centers with excellent regioselectivity.

Poster Presentation : **ORGN.P-587**

Organic Chemistry

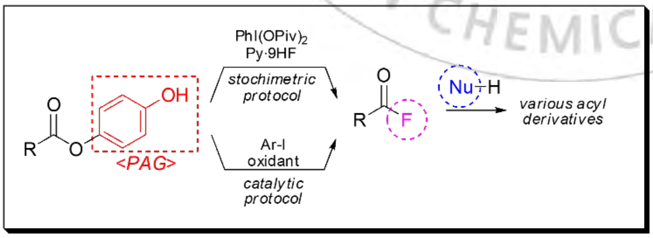
Event Hall FRI 11:00~13:00

Efficient Synthesis of Acyl Fluoride from Esters using Hypervalent Iodine(III)

Eunsol Choi, Hyo-Jun Lee*

Department of Chemistry, Kunsan National University, Korea

The development of efficient transformations of ester into various acyl derivatives is one of the most interesting research topic in modern organic chemistry. Synthesis of acyl fluoride, in particularly, is very attractive due to its synthetic utility. For example, various amides can be synthesized from nucleophilic acyl substitution of acyl fluorides with amines. Generally, acyl fluoride is obtained from carboxylic acid using fluorinating reagents such as cyanuric fluoride. However, generation of acyl fluoride from another acyl derivatives, such as amide, and ester, is rare. Here, we report a new acyl fluoride generation from 4-hydroxyphenol ester. 4-Hydroxyphenol, potential activating group (PAG), will be activated by hypervalent iodine(III) reagent and acyl fluoride will be generated by reaction with pyridine hydrogen fluoride complex under mild conditions. Furthermore, we are investigating catalytic protocol of ester activation using aryl iodide and certain oxidant.



Poster Presentation : **ORGN.P-588**

Organic Chemistry

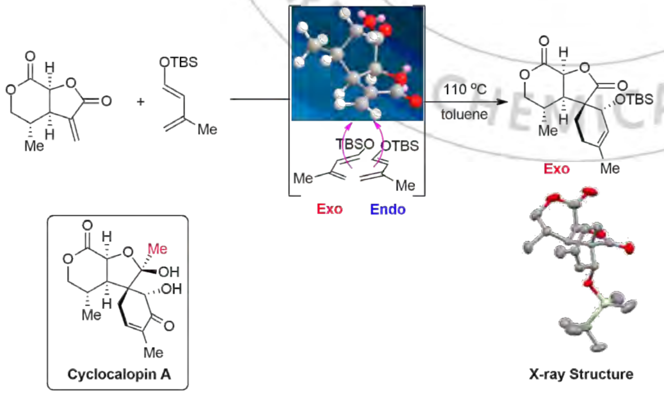
Event Hall FRI 11:00~13:00

A Construction of Spiro-ring Unit of Naturally Occurring Cyclocalopin A via Unusual Exo Diels–Alder Cycloaddition

Suh Young Yu, Hyeonjoung Choi, Seyeon Jung, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of transition metals are some of the most attractive methodologies since reactions can directly construct complicate molecules from relatively simple starting materials. The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. We have explored synthetic route from an allenyl glyoxylate to the tricyclic core skeletone of cyclocalopin A including an exo-selective Diels–Alder reaction of bis-gamma, delta-lactone. We would like to present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring cyclocalopin series: i. stereoselective elaboration of a spiro-system; ii. synthetic approach to cyclocalopin family.



Poster Presentation : **ORGN.P-589**

Organic Chemistry

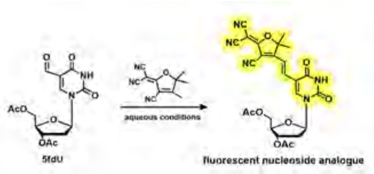
Event Hall FRI 11:00~13:00

Design and synthesis of fluorescent nucleoside analogues constructed by aldol-type condensation.

Hayeon Choi, Ki Tae Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

Fluorescent nucleosides have played essential roles in designs of functional nucleic acid systems for various biological applications (e.g. biosensors). In this context, developing novel fluorescent nucleosides featuring new functionalities has become an important challenge. Herein, we report novel fluorescent nucleosides based on aldol-type condensation between a 5-formyluracil and a dye with electron withdrawing groups. The newly designed fluorescent nucleosides were readily synthesized under mild organic conditions as well as under aqueous conditions, showing high conversion rates and reaction yields. Moreover, the synthesized fluorescent nucleosides were found to exhibit distinct green fluorescence attributed to a large stokes shift based on a push-pull type structure. In kinetic studies through HPLC, it was found that the reaction was completed within 8 hours under the condition of pH7 PBS aqueous solution. Such features of the fluorescence nucleosides were finally applied to selective fluorescent labeling of 5-formyluracil, known as an important target in epigenetics.



Poster Presentation : **ORGN.P-590**

Organic Chemistry

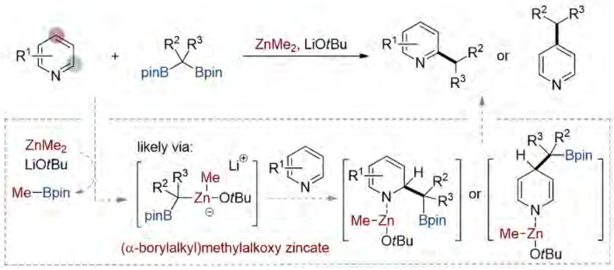
Event Hall FRI 11:00~13:00

The Reaction Development of ZnMe2-Mediated, Direct Alkylation of Electron-Deficient N-Heteroarenes with 1,1-Diborylalkanes

Woohyun Jo, Seung Hwan Cho*

Department of Chemistry, Pohang University of Science and Technology, Korea

Construction of carbon−carbon bonds is of central importance in synthetic chemistry. In particular, efficient and selective methods for the alkylation of simple electron-deficient N-heteroarenes, such as pyridines and quinolines, received much attention, in part because of the ubiquity of alkylated pyridines and quinolines in many natural products, pharmaceuticals, and agrochemicals. Herein, we report a ZnMe2-promoted, direct C2- or C4-selective primary and secondary alkylation of pyridines and quinolines using 1,1-diborylalkanes as alkylation sources. While substituted pyridines and quinolines exclusively afford C2-alkylated products, simple pyridine delivers C4-alkylated pyridine with excellent regioselectivity. The reaction scope is remarkably broad, and a range of C2- or C4-alkylated electron-deficient N-heteroarenes are obtained in good yields. Experimental and computational mechanistic studies imply that ZnMe2 serves not only as an activator of 1,1-diborylalkanes to generate (α-borylalkyl)methylalkoxy zincate, which acts as a Lewis acid to bind to the nitrogen atom of the heterocycles and controls the regioselectivity, but also as an oxidant for rearomatizing the dihydro-N-heteroarene intermediates to release the product.



Poster Presentation : **ORGN.P-591**

Organic Chemistry

Event Hall FRI 11:00~13:00

Strategic synthesis of fluorenones with acyl fluorides

Sung Pyo Youn, Hee Nam Lim[1,*]

Chemistry, Yeungnam University, Korea
[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

Fluorenone derivatives with diverse substitution patterns were synthesized by intramolecular Friedel-Crafts acylation using acyl fluorides as substrates. The synthetic method features mild, selective, and highly reactive system that uses two different preparation methods for key acyl fluorides.

Poster Presentation : **ORGN.P-592**

Organic Chemistry

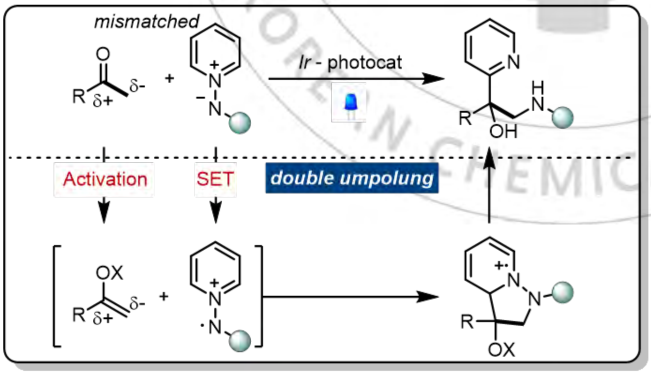
Event Hall FRI 11:00~13:00

Visible-Light-Induced 1,2-Aminopyridylation of Ketones via A Double Umpolung Strategy

Wonjun Choi, **Sungwoo Hong***

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Through a double umpolung strategy, 1,2-aminopyridylation of ketones with pyridinium N-N ylides as bifunctional reagent is developed. Polarity inversion is enabled by single-electron oxidation of N-N ylides and 1,3-dipolar cycloaddition with enolsilanes formed in situ from ketones and homolytic N-N bond cleavage can afford 1,2-aminopyridylated products. Intriguingly, two bonds are formed between positions of N-N ylides and ketones with the same electrical properties that are hard to access by their innate polarity-driven reactivity. A broad scope and biorelevant complex molecules are showed compatibility of this method.



Poster Presentation : **ORGN.P-593**

Organic Chemistry

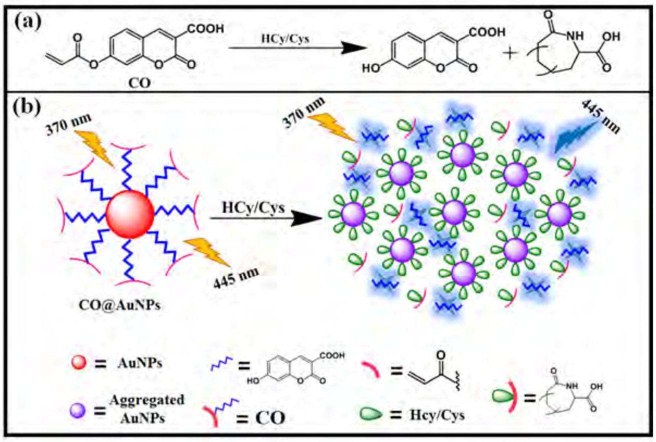
Event Hall FRI 11:00~13:00

Detection Time Based Selective Discrimination Of HCy From Cys Using Gold Nanoparticle Based Optical Probe And Its Application In Blood Plasma And Urine

Ratish Nair, Su Jin Na, Taemin Park[1], Seoung Ho Lee[1,*]

department of chemistry, Daegu University, Korea
[1]*Department of Chemistry, Daegu University, Korea*

Hyperhomocysteinemia (a clinical condition with increased homocysteine (Hcy) in human blood) is associated with various acute health disorders. Selective discrimination of HCy from Cys is very important. Consequently, Hcy measurement in human plasma is essential for clinical management of several vascular, cardiac, renal, and age related pathologies. Rapid detection of plasma Hcy by simple optical technique would be beneficial for clinical purpose. Moreover, sensitivity at physiological condition, cost of the reagents, and obligatory requirement of non-aqueous media have carried limitation to this endeavor. In the current work, synthesis and characterization of a new Hcy selective nanoparticle probe CO@AuNPs is reported. CO@AuNPs showed remarkable colorimetric and fluorimetric properties with Hcy in 100 % aqueous medium at physiological as well as at variable pH. The probe CO@AuNPs, discriminates HCy from Cys using detection time. The biosensor CO@AuNPs, with lower detection limit (LOD) of 120 nM can also be utilized for colorimetric detection of HCy in biological samples. Being non-toxic and permeable in nature, CO@AuNPs can function as a colorimetric staining reagent for HCy in biological samples. CO@AuNPs were validated for detection of HCy using HPLC technique. The probe CO@AuNPs can be used for detecting HCy in blood plasma and urine.


(a)
COOH
CO
HCy/Cys
HO
NH
OH
(b)
370 nm
445 nm
CO@AuNPs
HCy/Cys
= AuNPs
= Aggregated AuNPs
= CO
= Hcy/Cys

Poster Presentation : **ORGN.P-594**
Organic Chemistry
Event Hall FRI 11:00~13:00

Synthesis of 3-Sulfenylindoles under Photocatalytic Condition

Seunghoon Shin*, Chul Yong Lee[1]

Department of Chemistry, Hanyang University, Korea
[1]*Department of Chemistry, Hanyang university, Korea*

3-Sulfenylindoles are found in many bioactive natural and medicinal compounds. Synthesis of this scaffold have been developed by vanadium-catalyzed oxidative sulfenylation of indoles with thiols under O_2,[1] iron-catalyzed sulfenylation of indoles with disulfides,[2] and photocatalytic reaction of indoles with thiols under air.[3] Unfortunately, however, these methods were ineffective with the production of alkyl thioethers. We recently reported that N-acyloxyindole could be employed as umpoled indoles in the cross-coupling with phenols.[4] We posited that that the N-acyloxyindoles could be employed in the selective sulfenylation including alkyl thioethers.

Herein, we describe two recently discovered photocatalytic conditions for direct C3-sulfenylation of umpoled-2-phenylindole with both aryl and alkyl thiols as the sulfenylating agents. Under the irradiation of blue LEDs employing $Ru(bpz)_3$ as the photocatalyst, N-acyloxyindole derivatives underwent efficient sulfenylation with aromatic thiols at C3. The working hypothesis involves energy transfer (EnT) to form a carboxy radical, formation of a thiyl radical, and its addition into a N-acyloxyindole. Unfortunately, aliphatic thiols with higher S-H bond strength, gave poor yields and alternative conditions were developed. For aliphatic thiols, UV photolysis in the absence of catalyst gave good yields of the corresponding products.

References

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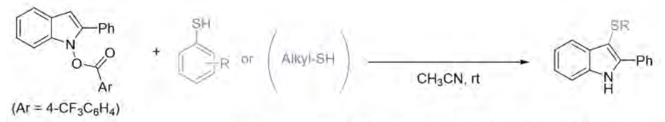
2. Tudge, M,; Tamiya, M.; Savarin, C.; Humphrey, G. R. *Org. Lett.* **2006**, 8, 4, 565–568.
3. (a) Fang, X.-L.; Tang, R.- Y.; Zhong, P.; Li, J. –H. *Synthesis* **2009**, 24, 4183-4189. (b) Guo, W.; Tan, W.; Zhao, M.; Tao, K.; Zheng, L.-Y.; Wu, Y.; Chen, D.; Fan, X.-L. *RSC Adv.*, **2017**, 7, 37739-37742.
4. (a) Oh, S. M. ; Shin, S. *Bull. Korean Chem. Soc.* **2021**, 42, 925-927. (b) Nguyen, N. H.; Oh, S. M.; Park, C.-M.; Shin, S. *Chem. Sci.* **2022**, 13, 1169-1176.



condition A : Ru(bpz)$_3$(PF$_6$)$_2$ (5 mol%), blue LEDs (450 nm, 18 W)
condition B : UV LEDs (405 nm, 18 W)

Poster Presentation : **ORGN.P-595**

Organic Chemistry

Event Hall FRI 11:00~13:00

Hollow Silica-magnetic Nanoparticles for External Stimuli-responsive Anti-cancer Drug Delivery

Ji-Hye Kang, Ueon Sang Shin[1,*]

Department of Nanobiomedical Science & BK21 PlUS NBM Global Research Center for Regenerative Medicine, Dankook University, Korea

[1]*Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Korea*

In present study, the focus is drawn towards the advantage of hollow core and uniformly distributed magnetic shell attributing to their invading property under magnetic field through the most abundant cancerous niche component; the collagen, while targeting breast cancer cells. Uniform monodispersed hollow silica nanospheres are synthesized and functionalized contributing the mesoporosity by a coating layer of poly(N-isopropylacrylamide-co-N-vinylimidazole-co-acrylic acid) (pNIBIm-AA) in the presence of magnetic nanoparticles (MNP). At 42 °C temperature (LCST) and/or low pH 5, the pNIBIm-AA/MSN/MNP shell undergoes a definite transition from open swollen state to collapse state; facilitating diffusion of loaded model drug Doxorubicin hydrochloride (DOX) in-and-out through pores of MSN channels. The pH-temperature dependent “turn-on/off” regulation of porous channels control the drug loading-release capacity of the particle; exhibiting approximate 17.5 % drug embedding efficiency. The pathological features of cancer is associated with low pH at tumor micromilieu; herein, attributes in control release of therapeutics from carrier at cancer niche. Considerably high cytotoxicity is experienced by human breast adenocarcinoma cells (MCF7) treated with DOX-particle at 42 °C compared to 37 °C, while virtually non-toxic to untreated cells; indicative of stimuli-responsive release of loaded drug from the particles apparently. The remarkable feature of the fabricated nanomaterials, thereby, compromises between pH-temperature sensitivity imparted by pNIBIm-AA and deep tissue invading property of magnetic nanoparticles to eradicate specific delivery of therapeutic molecules using standard equipment like MRI; causing minimal toxic side-effects for host.

Poster Presentation : **ORGN.P-596**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fluorescence turn-on sensor based on protamine-induced self-assembly for real-time monitoring of trypsin activity in human urine

Taemin Park, Minwoo Han, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

In this study, an effective fluorescence strategy for trypsin was developed by micelle-based fluorescence system on the protamine-caused quenching of pyrene derivatives. Water-soluble pyrene derivatives showing strong fluorescence are aggregated by protamine, resulting in amplified quenching. The addition of trypsin catalyzes the hydrolysis of protamine, which induces the disaggregation of the aggregated pyrene derivatives, thereby restoring strong fluorescence again. Based on this strategy, we have demonstrated highly sensitive and selective detection of trypsin, as well as the screening of trypsin inhibitors that are essential for drug discovery.

Poster Presentation : **ORGN.P-597**

Organic Chemistry

Event Hall FRI 11:00~13:00

Sensitive detection of trypsin activity in human urine using Protamine-induced self-assembly of TPE derivatives

Haemin Choi, Hyoyun Jang, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Trypsin is one of the digestive enzymes and is associated with pancreatic diseases such as pancreatic ileus and pancreatitis. To detect it with high selectivity and sensitivity, we have developed a novel fluorogenic detection system based on protamine-induced self-assembly of tetraphenyl ethylene (TPE) derivatives with water-soluble groups. Protamine induces supramolecular self-assembly of water-soluble TPE derivatives by electrostatic interaction and π–π stacking, resulting in a drastic fluorescence enhancement via aggregation induced emission (AIE). This system can efficiently detect the activity of trypsin via fluorescence quenching, where TPE aggregates are degraded by hydrolysis of protamine into fragments. This study has proven to be a sensitive and selective detection method not only for trypsin, but also for human urine and the screening of trypsin inhibitors, which are essential for the discovery of new drugs.

Poster Presentation : **ORGN.P-598**

Organic Chemistry

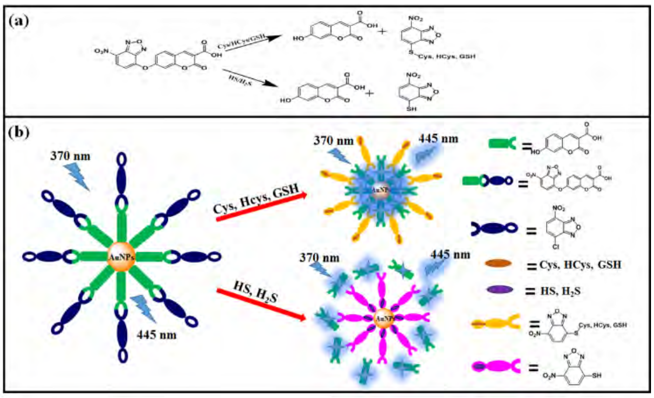
Event Hall FRI 11:00~13:00

NBD based Gold Nano particles for Detection of Biothiols and Their Selective Discrimination at varied pH conditions

Su Jin Na, **Ratish Nair**, **Seoung Ho Lee***

Department of Chemistry, Daegu University, Korea

Biothiols are associated with different physiological and pathological processes, while abnormal levels of biothiols are related to several disorders. It is crucial to discriminatively identify these molecules and discover their inherent alteration in living biological samples. In our work we have utilised the thiolysis of NBD amines for the development of probe that can selectively discriminate between biothiols (HS, H2S, Cys, HCys and GSH. NBD amine is coupled with coumarin moiety and is embedded on the surface of gold nanoparticles to form a new probe CONBD@AuNPs. The probe CONBD@AuNPs shows both effective colorimetric and fluorescence enhancement detection of biothiols. CONBD@AuNPs can selectively discriminate between using HS, H2S, Cys, HCys and GSH colorimetric technique. Using CONBD@AuNPs the biothiols can be detected at different pH in the range 3 to 9.The probe can detect very low levels of HS and H2S and hence, can be used for imaging and detection in different biological samples. CONBD@AuNPs can also be used to showcase the potential to verify the biosynthesis of endogenous H2S from Cys.



Poster Presentation : **ORGN.P-599**

Organic Chemistry

Event Hall FRI 11:00~13:00

Therapeutic tissue regenerative nanohybrids self-assembled from bioactive inorganic core / chitosan shell nanounits

Han Sem Kim

Institute of Tissue Regeneration Engineering, Dankook University, Korea

Natural inorganic/organic nanohybrids are a fascinating model in biomaterials design due to their ultramicrostructure and extraordinary properties. Here, we report unique-structured nanohybrids through selfassembly of biomedical inorganic/organic nanounits, composed of bioactive inorganic nanoparticle core (hydroxyapatite, bioactive glass, or mesoporous silica) and chitosan shell - namely Chit@IOC. The inorganic core thin-shelled with chitosan could constitute as high as 90%, strikingly contrasted with the conventional composites. The Chit@IOC nanohybrids were highly resilient under cyclic load and resisted external stress almost an order of magnitude effectively than the conventional composites. The nanohybrids, with the nano-roughened surface topography, could accelerate the cellular responses through stimulated integrin-mediated focal adhesions. The nanohybrids were also able to load multiple therapeutic molecules in the core and shell compartment and then release sequentially, demonstrating controlled delivery systems. The nanohybrids compartmentally loaded with therapeutic molecules (dexamethasone, fibroblast growth factor 2, and phenamil) were shown to stimulate the anti-inflammatory, pro-angiogenic and osteogenic events of relevant cells. When implanted in the in vivo calvarium defect model with 3D-printed scaffold forms, the therapeutic nanohybrids were proven to accelerate new bone formation. Overall, the nanohybrids self-assembled from Chit@IOC nanounits, with their unique properties (ultrahigh inorganic content, nano-topography, high resilience, multiple-therapeutics delivery, and cellular activation), can be considered as promising 3D tissue regenerative platforms.

Poster Presentation : **ORGN.P-600**

Organic Chemistry

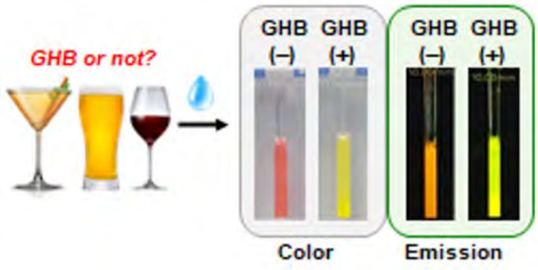
Event Hall FRI 11:00~13:00

Metal Complexes for Rapid Colorimetric and Fluorescent Detection of Date-Rape Drug gamma-Hydroxybutyrate

Junghyun Ryu, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

Gamma-Hydroxybutyrate (GHB) is a colorless and odorless type of drug. We will present a simple colorimetric and fluorimetric indicator for the rapid and sensitive determination of GHB. To design a chemosensor for the detection of illicit date-rape drug GHB, we explored the displayed spectral response of the metal complexes based on its complexation and decomplexation with Fe(III) ions. Assays were developed to detect the presence of GHB in spiked alcoholic and non-alcoholic beverages in both solution and practical solid-state indicator strips. The metal complexes have high stability and changes color from red-pink to yellow under the conditions of the GHB. On the other hand, there is no color change in various pH buffers under the assay condition without GHB. Based on the rapid color changes, the metal complexes solution assay can detect the presence of GHB within 5 seconds. We anticipate that the metal complexes can be applied as a valuable analytical tool to help prevent GHB-related drug-facilitated sexual assault.



129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-601**

Organic Chemistry

Event Hall FRI 11:00~13:00

Pd-Catalyzed Regioselective Intramolecular Allylic C-H Amination of Labile Allyl Ethers

Dongbin Kim, So Won Youn*

Department of Chemistry, Hanyang University, Korea

We report the Pd-catalyzed intramolecular allylic C-H amination of 1,1-disubstituted alkenyl amines with various allylic tethers to afford diverse 5-membered 1,3-*X*,*N*-heterocycles with excellent chemo- and regioselectivity through allylic C−H cleavage/π-allylpalladium formation. Particularly noteworthy is the use of substrates containing a labile allylic moiety and new simple catalytic systems capable of promoting highly chemo- and regioselective allylic C-H amination by overcoming significant challenges.

Poster Presentation : **ORGN.P-602**

Organic Chemistry

Event Hall FRI 11:00~13:00

Ag-Catalyzed Tandem Olefin Isomerization/Intramolecular Hydroamination of Allyl Ethers, Amines, and Sulfides

Dongbin Kim, So Won Youn*

Department of Chemistry, Hanyang University, Korea

Five-membered *N*-heterocycles containing 1,3-diheteroatoms (e.g., oxazolidines, imidazolidines, thiazolidines) frequently found in natural products and pharmaceuticals exhibit a diverse range of biological activities and are broadly applicable in synthetic, medicinal, and polymer chemistry. We report the Ag-catalyzed tandem olefin isomerization/intramolecular hydroamination of alkenyl amines with various allylic tethers to afford diverse 5-membered 1,3-*X*,*N*-heterocycles. In sharp contrast to the related prior works, simple and readily accessible catalysts, reagents, and reactants are used under mild aerobic conditions.

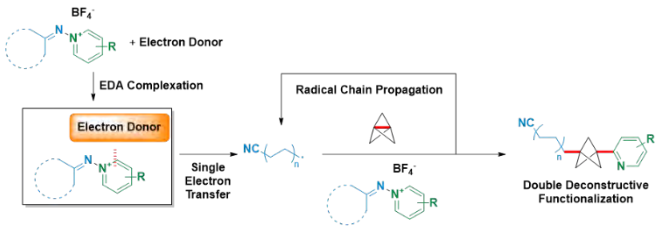
Poster Presentation : **ORGN.P-603**
Organic Chemistry
Event Hall FRI 11:00~13:00

Electron Donor-Acceptor Complex Promoted Direct Difunctionalization of Tricyclo[1.1.1]pentane

Seunghyun Lee, Eun Joo Kang[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Recently, functionalization of tricyclo[1.1.1]pentane(TCP) is significantly spotlighted because bicyclo[1.1.0]pentane(BCP) scaffolds from TCP are able to replace functional groups such as alkynl, aryl and tert-butyl in various pharmaceuticals and natural compounds with enhanced chemical and pharmacological properties (metabolic tolerance, bioactivity etc). Therefore, a plenty of researches on BCP functionalizing are actively on going[1], however direct C,C-difunctionalization of TCP is still in the dark side. Herein, we designed novel imino-pyridinium substrate which can be cleaved under reductive single electron transfer by electron donor-acceptor complexation and generate iminyl radical which have strong ring strain energy. Iminyl radical intermediate is able to form alkyl radicals by β-scission[2] then alkyl radical intermediates finally react with TCP to form functionalized BCP. The whole reaction process goes on radical chain process and subsequent mechanistic studies and substrate expansions are still on going. **Acknowledgement**This study was supported by the Ministry of Education, science and Technology, National Research Foundation (Grant Numbers NRF-2021R1A2C1013993).**References**1. Pickford, H. D.; Nugent, J.; Owen, B.; Mousseau, J. J.; Smith, R. C.; Anderson, E. A. *J. Am. Chem. Soc.* **2021**, 143, 9729-9736.2. Ai, W.-Y.; Liu, Y.-Q.; Wang, Q.; Lu, Z.-L.; Liu, Q. *Org. Lett.* **2018**, 20, 409−412.



Poster Presentation : **ORGN.P-604**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of tetrasubstituted α,β-unsaturated ketones through Oppenauer oxidation with alkenylmagnesiums and aldehydes

Hwiwoong Lee, Yunmi Lee[1,*]

Chemistry, Kwangwoon University, Korea

[1]*Department of Chemistry, Kwangwoon University, Korea*

Oppenauer oxidation is one of the most useful and mild methods for converting alcohols into ketones. This form of oxidation was suggested to proceed by transfer of the hydride of metal alkoxide intermediates to the aldehyde. Aluminum alkoxides as well as various metal alkoxides including magnesium, zinc, tin, indium and zirconium metals are involved in this transformation. In this study, we describe the use of magnesium alkoxides derived from the nucleophilic addition of an alkenylmagnesium reagent to an aldehyde to achieve Oppenauer oxidation. Nickel-catalyzed carbomagnesation of internal alkynes using readily available arylmagnesium reagents generated trisubstituted alkenylmagnesiums, which were added to the aldehyde followed by Oppenauer oxidation. This protocol allowed for one-pot synthesis of new and versatile tetrasubstituted α,β-unsaturated ketones with high yields.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ORGN.P-605**

Organic Chemistry

Event Hall FRI 11:00~13:00

Solution Processable Benzo[b]thieno[2,3-d]thiophene Derivatives as Small Molecular Organic Semiconductors for Organic Thin-Film Transistors

Soomin Ryu, Sungyong Seo[1,*]

Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

Newly synthesized benzo[b]thieno[2,3-d]thiophene derivatives, 2-([2,2’-bithiophene]-5-yl)benzo[b]thieno[2,3-d]thiophene (1), 2-(5’-(2-ethylhexyl)-[2,2’-bithiophene]-5-yl)benzo[b]thieno[2,3-d]thiophene (2), and 2-(5’-octyl-[2,2’-bithiophen]-5-yl)benzo[b]thieno[2,3-d]thiophene (3), were employed as organic semiconductors (OSCs) via solution process for organic thin film transistors (OTFTs). Three organic compounds were characterized by thermogravimetric analysis (TGA), differential scanning calorimeter (DSC), cyclic voltammetry (CV), UV-visible spectroscopy, and density functional theory (DFT) calculation. Solution-shearing (SS) method was used to form thin films of the compounds, and microstructure as well as morphology of the thin films were investigated with atomic force microscopy (AFM) and θ-2θ X-ray diffraction (XRD). Fabricated OTFTs based on thin films of each compound exhibited p-channel activity in ambient condition, and especially transistors based on compound 2 featured hole mobility up to 0.057 cm^2/Vs and current on/off ratio over 10^7, in accordance with thin films of compound 2 showing superb surface coverage and high film texture.

Poster Presentation : **ORGN.P-606**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis and Evaluation of 6-Benzo[b]thiophene Derivatives for Organic Thin-Film Transistors(OTFTs)

JiHae Ahn, Sungyong Seo*

Department of Chemistry, Pukyong National University, Korea

6-Benzo[b]thiophene derivatives, 6-(5-octylthiophen-2-yl)-2-(thiophen-2-yl)benzo[b]thiophene and 2,6-bis(5-octylthiophen-2-yl)benzo[b]thiophene, were designed and synthesized for application in organic thin-film transistors(OTFTs). To evaluate the performance of OTFTs fabricated using 6-benzo[b]thiophene-derivatives, the thermal, optical, electrochemical, and electrical properties were investigated. The resulting OFETs based on films of 6-(5-octylthiophen-2-yl)-2-(thiophen-2-yl)benzo[b]thiophene showed the highest hole mobility of 0.038 cm^2/Vs and current on/off ratio of 1.2 × 10^7.

Poster Presentation : **ORGN.P-607**

Organic Chemistry

Event Hall FRI 11:00~13:00

An asymmetric conjugated oligomer based on 5-benzo[b]thiophene for organic thin-film transistors

<u>YuSeong Kim</u>, Sungyong Seo[1,*]

Chemistry, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

Novel 5-benzo[b]thiophene derivatives, 2,5-bis(5-octylthiophen-2-yl)benzo[b]thiophene was synthesized and characterized as solution-processable organic thin-film transistors (OTFT). To investigate the thermal, optical, electrochemical, and electrical properties of newly synthesized 5-benzo[b]thiophene derivative, active layer/insulator layer OTFTs was fabricated and characterized in ambient conditions. This compound exhibited p-channel activity, the resulting OTFTs based on films of 2,5-bis(5-octylthiophen-2-yl)benzo[b]thiophene showed hole mobility of 0.003 cm2/Vs and current on/off ratio of 9.3 × 105.

Poster Presentation : **ORGN.P-608**

Organic Chemistry

Event Hall FRI 11:00~13:00

Boryl Aminoaryne Precursors: Versatile Building Blocks for Aminoarenes

EunHye Ju[*], Young-Kyo Jeon, Won-SuK Kim[1,*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea

[1]*Chemistry Department of Nano-Science, Ewha Womans University, Korea*

Boryl aminoaryne precursors were efficiently synthesized from 3-aminobenzyne precursors via *meta*-selective iridium-catalyzed C-H borylation for the synthesis of various aminoarene derivatives. Palladium-catalyzed Suzuki-Miyaura cross coupling reactions of the boryl aminoaryne precursors with aryl halides were achieved well to access *meta*-arylated aminobenzyne precursors, which are induced by C-(sp^2)-to-N 1,3-aza-Brook rearrangement. Further functionalization of primary amine or pinacol boronic ester groups of the boryl aminoaryne precursors was also accomplished, respectively. Finally, to demonstrate the practical convenience, a one-pot two-step synthesis of 3,5-disubstituted and 2,3,5-trisubstituted aminoarenes starting from boryl aminobenzyne precursors was performed.

Poster Presentation : **ORGN.P-609**

Organic Chemistry

Event Hall FRI 11:00~13:00

Pd-Catalyzed Ortho Arylation of (Hetero) Aryl Tosylates

Yong-Ju Kwon, Inji Shin[1], Won-SuK Kim[2,*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Seoul National University of Science & Technology, Korea*
[2]*Chemistry Department of Nano-Science, Ewha Womans University, Korea*

Pd-catalyzed regioselective ortho arylation of (hetero) aryl tosylates has been investigated using an integrated continuous flow and batch protocol. Continuous flow ortho metalation of (hetero)aryl tosylates using *n*-BuLi and $ZnCl_2$ was successfully achieved while inhibiting the formation of (hetero) aryne intermediate. Pd-catalyzed Negishi coupling reactions of arylzinc species with various aryl iodides proceeded well at room temperature. Finally, with this method, an anti-epileptic drug, perampanel was successfully synthesized in linear four steps from 3,5-dibromo-2-hydroxy pyridine.

Poster Presentation : **ORGN.P-610**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis, opto-physical properties, and theoretical studies of dithieno[3,2-b:2’,3’-d]thiophene and diseleno[3,2-b:2’,3’-d]thiophene derivatives

Kyukwan Zong*, Hwanhee Jo

Department of Chemistry Education, Jeonbuk National University, Korea

Fused conjugated heterocycles such as dithienothiophene and diselenothiophene have received a great attention as an organic semiconductor for applications to a broad spectrum of organic electronics. Recently, thienothiophenes or dithienothiophenes successfully applied to fused-nonfullerene acceptors as a donor unit and greatly contributed to boost organic solar cell efficiency. We developed a highly efficient synthetic routes, carried out opto-physical studies, and theoretical study based on DFT calculations. Interestingly, the selenium analog substituted with p-tert-butylphenyl shows much red-shifted λmax (387 nm) than sulfur analog does (373 nm). The bandgaps of both compounds based on these optical properties were determined as 2.88 eV and 2.97 eV respectively. In addition, the onset oxidation potentials (Eoxonset) of both compounds derived from the cyclovoltammograms were measured as 1.10 eV and 1.26 eV, respectively, which is well agreed with the optical properties observed from these compounds. DFT calculations reveals that the fused cores of both systems are highly plated and well-delocalized HOMO orbitals of the conjugated π systems. Synthetic details, optical & electrochemical studies, and the results of DFT calculations will be described in this presentation.


S
R
S
S
R
R = H, alkyl, aryl,
heteroaryl


S
R_1
Se
Se
R_1
R_1 = aryl, heteroaryl

Poster Presentation : **ORGN.P-611**

Organic Chemistry

Event Hall FRI 11:00~13:00

Visible-Light Photocatalytic Deoxygenation of Amine N-Oxides With Hantzsch Esters as Mild Reducing Agents

Ju Hyeon An, HoKyeong Ryu, Jun Hee Lee[1,*]

Department of Chemistry, Dongguk University, Korea

[1]*Department of Advanced Materials Chemistry, Dongguk University, Korea*

Herein, we disclose a highly chemoselective room-temperature deoxygenation method applicable to variousfunctionalized amine *N*-oxides via visible light-mediated photoredox catalysis using Hantzsch esters as the sole stoichiometric reductant. Most of these deoxygenations can be completed within a few minutes or hours using metalla- or oranophotocatalysts, respectively. These technologies also allow multigram-scale reactions even with an extremely low catalyst loading. The scope of this scalable and operationally simple protocol encompasses a wide range of functional groups, such as amides, carbamates, esters, ketones, nitrile groups, nitro groups, and halogens, which provide access to the corresponding deoxygenated amines in good to excellent yields.

Poster Presentation : **ORGN.P-612**
Organic Chemistry
Event Hall FRI 11:00~13:00

Study on Improve Lightfastness of High Visibility Rhodamine Based Colorant materials

Hyeon Oh, Si Hyeong Park, MinWoo Han, Wonbin Kim, Hyunseo Kim, Young-A Son[1,*]

Organic Materials Engineering, Chungnam National University, Korea
[1]*Dept. of Advanced Organic Materials Engineering, Chungnam National University, Korea*

With the rapid growth of the industry, we have faced safety problems such as fires and accidents. Interest in safety has brought about the demand for protective clothing, and high-visibility fluorescent dyes on protective clothing have become a very important factor in protecting workers in industrial sites. Rhodamine is a high visibility fluorescent material and is widely used for its excellent characteristics such as high quantum efficiency, molar absorption coefficient, and narrow absorption wavelength. However, high-visibility materials that have been dyed show limitations in lightfastness. Therefore, we devised a method to increase the lightfastness of rhodamine. First, an ultraviolet absorber was introduced. The ultraviolet absorber absorbs ultraviolet rays and converts them into thermal energy, and repeats reduction to prevent ultraviolet rays. In another way, a rigid structure was introduced. The rigid structure is packing the molecular structure to increase lightfastness. This experiment confirmed the improvement of lightfastness by comparing each rhodamine with ultraviolet absorber and rigid rhodamine with common rhodamine. In addition, lightfastness was confirmed by dyeing the modacrylic fiber with excellent flame retardancy.

Poster Presentation : **ORGN.P-613**
Organic Chemistry
Event Hall FRI 11:00~13:00

Synthesis of Reactive Disperse Dyes for Nylon and Cotton Substrates in Supercritical Dyeing Condition

Si Hyeong Park, Hyeon Oh, MinWoo Han, Wonbin Kim, Young-A Son*

Dept. of Advanced Organic Materials Engineering, Chungnam National University, Korea

In the traditional aqueous dyeing method, the dyeing of 1 kg of synthetic or natural fibers required approximately 100–145 L of water and also excessively used various chemical additives to dissolve dyes in the dyeing process. This method produces a large amount of wastewater which has a serious carcinogenic effect on aquatic lives and is also harmful to the environment. The purification of wastewater by ultrafiltration and sorption methods could give nearly 100% pure water. However, these purifications are always a considerable concern for economic aspects. Moreover, water is a finite resource. Therefore, the textile industry looking for a greener dyeing method to substitute the existing water dyeing method. The supercritical fluid dyeing (SFD) process is attracted in both economic and ecological aspects. In this study, we focus on the synthesis of reactive disperse dyes for dyeing polyamide and cotton fabrics in the supercritical fluid to respond to this eco-friendly aspect.

Poster Presentation : **ORGN.P-614**

Organic Chemistry

Event Hall FRI 11:00~13:00

Study on Colorants to Improve the Physical Properties of Aqueous Based Ink Formulation

MinWoo Han, Si Hyeong Park, Hyeon Oh, Wonbin Kim, Young-A Son[1,*]

Organic Materials Engineering, Chungnam National University, Korea

[1]*Dept. of Advanced Organic Materials Engineering, Chungnam National University, Korea*

Recently, as environmental problems increase, eco-friendly materials are becoming important. Accordingly, interest in eco-friendly ink materials is also increasing. Commercially used solvent ink is inexpensive, Although commercially used solvent ink is inexpensive, there is a problem in that volatile organic compounds (VOCs) that are harmful to the human body are released. As an alternative to this, aqueous ink is attracting attention as an eco-friendly ink material because a solvent is not used. There are still many problems than solvent ink, such as durability, adhesion, and color development to aqueous ink. To improve this problem, we predicted physical properties using computational chemistry (ðSystems, Dmol3, Gaussian, DFT calculations) for commercially available water dispersion ink materials. In addition, the possibility of modifying the basic structure was confirmed and a new molecular structure was designed.

Poster Presentation : **ORGN.P-615**

Organic Chemistry

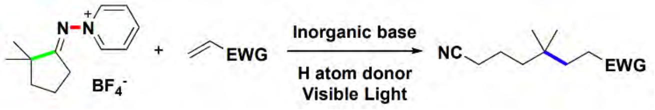
Event Hall FRI 11:00~13:00

Deaminative Ring Opening of Iminopyridinium Salts via Photoinduced Single-Electron Transfer

Gyuri Han

Department of Applied Chemistry, Kyung Hee University, Korea

Cyclic oximes can generate iminyl radicals through homolytic N-O bond cleavage and iminyl radicals can be used as effective precursor for alkyl radicals with terminal nitrile functional group by ring opening. While cyclic oximes have many variables in homolytic cleavage and regulates the diversity owing to the polarized N-O bond, in this work, N-N bond cleavage approach instead of N-O bond cleavage is designed to induce divergent transformation reactions. The electron deficient iminopyridine salts are used as electron acceptor for Electron donor acceptor complex (EDA complex) and inorganic bases such as K_2CO_3, Cs_2CO_3, K_3PO_4 are employed as electron donor to make EDA complex. By irradiating visible light to EDA complex, intermolecular single electron transfer occurs[1] and iminyl radical is generated through homolytic N-N bond cleavage. Corresponding iminyl radical is transformed to terminal alkyl radical by the deconstructive ring opening pathway and the alkyl radical is added to α, β-unsaturated Michael acceptor. Therefore, the novel radical reaction using EDA complex with inorganic base successfully proceeds under mild reaction condition without any metal catalyst and oxidants. Acknowledgement This study was supported by the Ministry of Education, science and Technology, National Research Foundation (Grant Numbers NRF-2021R1A2C1013993, 2021R1A4A1030449). References 1. Giacomo E. M. Crisenza.; Daniele Mazzarella.; Paolo Melchiorre, *J. Am. Chem. Soc.* **2020**, 142, 5461−5476.



Poster Presentation : **ORGN.P-616**

Organic Chemistry

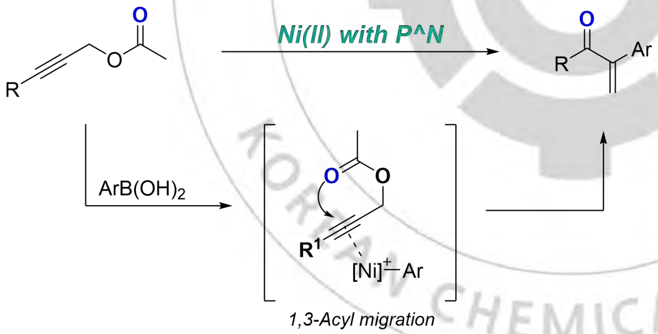
Event Hall FRI 11:00~13:00

Ni-Catalyzed Meyer-Schuster reaction with P^N ligand

Woo In Lee, Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

We report a Ni-Catalyzed Meyer-Schuster reaction of propargyl acetates to give α, β-unsaturated ketones through 1,3-acyl migration. With a bidentate P^N ligand, ^{i}PrPHOX, Ni complex shows Lewis acidic alkynophilic reactivity similar to those of late 5d-metals, such as gold and platinum. The astonishing alkynophilic character of the Ni(II)/P^N system was supported by a series of experimental and computational studies.



Poster Presentation : **ORGN.P-617**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of Acridine-Based High Visibility Fluorescent Molecules Towards TPU

Wonbin Kim, Si Hyeong Park, Hyeon Oh, MinWoo Han, Young-A Son*

Dept. of Advanced Organic Materials Engineering, Chungnam National University, Korea

As the global environment and resource conservation and conservation issues emerged, international efforts to improve environmental pollution began, including regulations on global environmental pollution, carbon emission reduction, and waste reduction policies around the world. Among these, research on the manufacture of solvent-free, eco-friendly biomass-based thermoplastic polyurethane (TPU) fibers that do not use solvents is also being actively conducted. Color problems occur as the biomass content increases. This study aimed at the molecular structure design, simulation, and synthesis technology development of fluorescent materials using acridine derivatives applicable to TPU materials. PPP-MO π-systems, Dmol³, DFT calculation The color absorption and fluorescence wavelength of the newly designed acridine dye were calculated using computational chemistry software, and the molecular structure synthesis with improved visibility was studied. In addition, it was confirmed whether TPU can be applied to a novel high-visibility acridine material by using a UV-vis device.

Poster Presentation : **ORGN.P-618**

Organic Chemistry

Event Hall FRI 11:00~13:00

Half Sandwich Metal-Mediated Tail-to-Tail Homocoupling of Terminal Ynamides through Dual Activation Mode of Triple Bonds

Sourav Pradhan, Sukbok Chang[1,*]

Department of Chemistry, Institute for Basic Science, Korea

[1]*Department of Chemistry, Institute for Basic Science (IBS) / Korea Advanced Institute of Science and Technology, Korea*

Half-sandwich metal-mediated an unprecedented tail-to-tail homocoupling of terminal N-sulfonyl and N-acyl ynamides is described to furnish dienyl bisamido metal-complexes via a dual activation mode of alkynes. The alkenyl metal complexes are well characterized by ^{1}H, ^{13}C NMR and X-ray crystallographic techniques. This transformation was shown to be compatible with piano-stool Rh, Ru and Ir complexes. The mechanistic underpinnings are realized based on DFT calculations and the reaction was proposed to proceed via a dual activation mode of the triple bonds: (i) generation of a zwitterionic keteniminyl metal species to prompt an intramolecular chloride transfer and (ii) syn-carbometallation of the second coordinated alkynes by the alkenyl metal intermediate. The cyclic voltammetry analysis of a dienyl bisamido rhodacyclic complex guided to envision their possible oxidative modifications. Thus, protodemetallation, deuteration, iodination and acetoxylation of the Rh-dienyl complex is achieved under mild conditions.

Poster Presentation : **ORGN.P-619**

Organic Chemistry

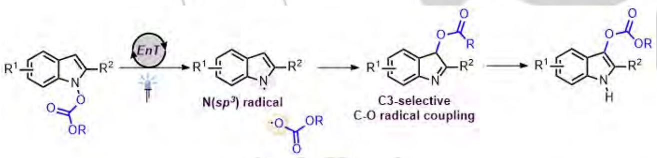
Event Hall FRI 11:00~13:00

Energy Transfer Photocatalytic Radical Rearrangement in N-Indolyl Carbontes

Ho Seong Hwang, Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

A new type of sp3-like N-centered radical has been generated by selective energy transfer catalysis. Upon photoexcitation, homolytic N−O bond cleavage of N-indolyl carbonate in the presence of an Ir-complex produced N- and O-centered radicals. The high spin density at the C3 position of indole led to radical recombination with O-centered radical, affording valuable 3-oxyindole derivatives without decarboxylation. Transformations of desired products into various molecules were also demonstrated.



Poster Presentation : **ORGN.P-620**

Organic Chemistry

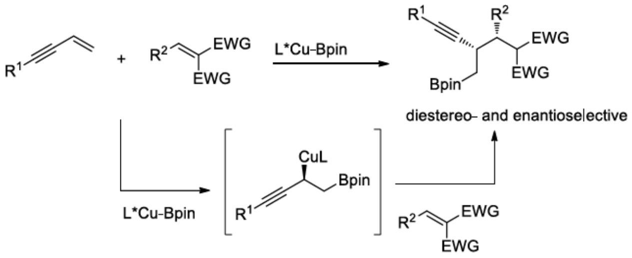
Event Hall FRI 11:00~13:00

Copper-Catalyzed Asymmetric Borylative Coupling of Terminal Enynes with Conjugated Diesters

Wan seok Yoon, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

We recently reported copper-catalyzed conjugative addition of alkylcopper nucleophiles to Michael acceptors, resulting in enantioselective formation of C(sp3)–C(sp3) bond with a single stereocenter. However, further attempts to increase the steric bulk of the alkylcopper-nucleophile derivatives from primary to secondary were not successful. Herein, we successfully developed an efficient asymmetric catalytic methods that employ two prochiral alkenes to form C(sp3)–C(sp3) bond with concomitant stereocontrol. In this work, we obtained the coupled product of 1,3-enynes and α,β-unsaturated diesters with high diastereo- and enantioselectivity.



Poster Presentation : **ORGN.P-621**

Organic Chemistry

Event Hall FRI 11:00~13:00

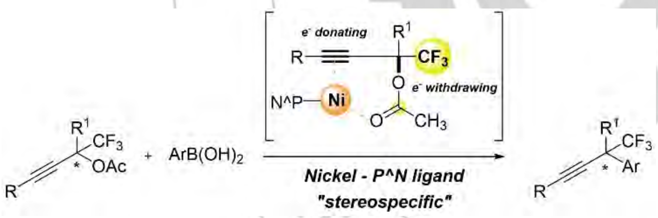
Ni-catalyzed substitution process of propargyl tertiary acetates

<u>Seo Yeon Kim</u>, Eun Jin Cho[1,*]

Chemistry, Chung-Ang University, Korea

[1]*Department of Chemistry, Chung-Ang University, Korea*

We have developed a Ni-catalyzed stereospecific substitution process of propargylic tertiary substrates. The ligand choice was critical for the efficiency and selectivity of the process where only bidentate P^N ligand promoted the process for the construction of new C–C bond. The use of leaving group coordinating to Ni-complex was also critical for the reactivity and selectivity of the process.



Poster Presentation : **ORGN.P-622**

Organic Chemistry

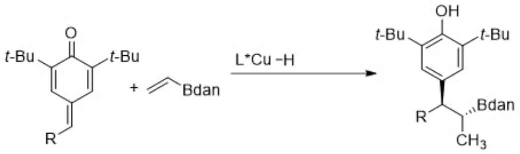
Event Hall FRI 11:00~13:00

Copper-Catalyzed Reductive Coupling of Borylalkenes And para-Quinone Methides

Meng Deyuan, He Jing, Jaesook Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Copper-catalyzed 1,6-addition reaction of borylalkene-derived nucleophiles to para-quinone methides (p-QMs) was described. This method is a successful protocol of constructing diaryl compounds containing two continuous stereogenic centers using two π-substrates. In the presence of a chiral bisphosphine-CuH as catalyst, a chiral organoboron copper intermediate is formed from a boryl alkene via stereoselective hydrocurpration. Its conjugative addition to p-QMs produced chiral diaryl compounds in good yield with good diastereo-and enantioselectivity.



Poster Presentation : **ORGN.P-623**

Organic Chemistry

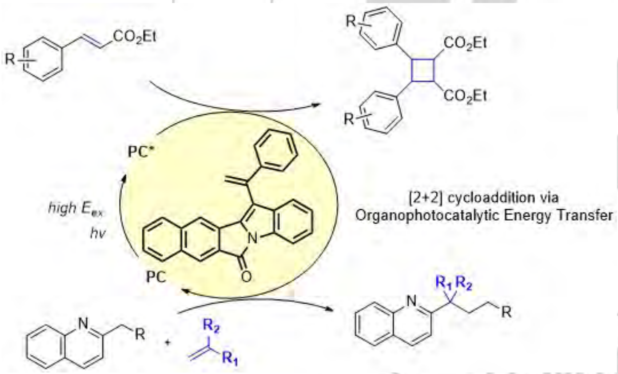
Event Hall FRI 11:00~13:00

Development of an indole-fused pentacyclic organophotocatalyst

Yunjeong Lee, **Eun Jin Cho***

Department of Chemistry, Chung-Ang University, Korea

We have synthesized an indole-fused conjugated pentacyclic complex which shows an excellent photophysical properties. It has been used as a good photocatalyst especially in energy transfer catalytic processes. In detail, we successfully applied the complex as PC in the following [2+2] cycloaddition, proving the utility of the developed complex.



Poster Presentation : **ORGN.P-624**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthesis of 2-(2-Nitroaryl)indole-3-acetic Acid Derivatives

Juhyeon Park, Cheol-Hong Cheon[*]

Department of Chemistry, Korea University, Korea

Since 2-aryl substituted indole-3-acetic acid derivatives have been utilized as the key subunits present in pharmaceuticals, natural products, agrochemicals, and other biologically active molecules, the development of a novel protocol to access these important building blocks has been consider the research of importance, and a number of synthetic protocols to access these building blocks have been reported. One of the straightforward methods to access these important building blocks would be intramolecular cyclization of N-benzyl-2-aminocinnamic acid derivatives followed by the oxidation. However, there have been no reports on the synthesis of 2-aryl indole-3-acetic acid derivatives from simple N-benzyl-2-aminocinnamic acid derivatives under basic conditions presumably due to inaccessibility of the carbanion at the benzylic position from N-benzyl-2-aminocinnamic acid derivatives. In this poster presentation, we will disclose a two-step protocol to access 2-(2-nitrophenyl)indole-3-acitic acid derivatives from N-(2-nitrobenzyl)-2-aminocinnamic acid derivatives. Treatment of N-(2-nitrobenzyl)-2-aminocinnamic acid derivatives with a base afforded benzylic anionic intermediates, which underwent cyclization to the neighboring unsaturated carbonyl moiety, leading to 2-(2-nitroaryl)indoline-3-acetic acid derivatives. Subsequent oxidation of the indoline to the indole scaffold provided 2-(2-nitroaryl)indole-3-acetic acid derivatives. Furthermore, the utility of this protocol was demonstrated in the concise total synthesis of paullone.

Poster Presentation : **ORGN.P-625**
Organic Chemistry
Event Hall FRI 11:00~13:00

Synthetic Studies towards Ngouniensine

Taewook Kim, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Ngouniensine, isolated and structurally determined in 1982, is one of the major indole alkaloids of Strychnos ngouniensis. Unlike other indole alkaloids, it has unusual structural features; ngouniensine is a tetracyclic scaffold and possesses 7-membered ring. In addition, ngouniensine has an exocyclic methylene group bridged to the C-2 position of the indole scaffold and the C-3 position. Furthermore, the two hydrogens at the C-3 and C-20 positions have a cis-relationship.The previous total synthesis of ngouniensine commenced with a starting material bearing the piperidine scaffold with the desired substituents and right stereochemistry. The indole was introduced by the SN2 reaction of the piperidine with tryptophyl bromide. Subsequent intramolecular Friedel-Crafts type reaction allowed the seven-membered ring formation. The final introduction of the methylene completed the synthesis of ngouniensine. However, this strategy generally required a lengthy sequence and the control of the stereochemistry was often challenging.In this poster presentation, a novel strategy proposal for the synthesis of ngouniensine will be presented. Pyridine containing substituents at the C-3 and C-20 positions was used as a surrogate for the key piperidine scaffold. Alkylation of ethenone compound with 2-aminocinnamate and ring formation afforded the corresponding indoline intermediate. Subsequent indolization will allow 2-(2-pyridylcarbonyl) indole-3-acetate. After that, through the condensation and reduction will be utilized as a precursor of the piperidine ring. Syn-selective reduction of the pyridinium ring will afford the piperidine ring with right stereochemistry, and the Wittig reaction of the carbonyl group to methylene group will complete the total synthesis of ngouniensine.

Poster Presentation : **ORGN.P-626**

Organic Chemistry

Event Hall FRI 11:00~13:00

Synthetic Studies towards Yohimbine Alkaloids

Jihyun Kang, Myunghoon Jeong[1], Cheol-Hong Cheon[1,*]

Chemistry, Korea University, Korea
[1]*Department of Chemistry, Korea University, Korea*

Yohimbine is one of the most well-known indole alkaloids with a rich chemical and medicinal history. The first total synthesis of the racemic compound was achieved more than 50 years ago by Van Tamelen and co-workers. Since the seminal synthesis, several other syntheses including asymmetric synthesis have been reported. Most previous syntheses of yohimbine commenced with a specific starting material containing the key fragment, the ester group and the hydroxyl group at the C-16 and C-17 positions with appropriate stereochemistry, respectively. Subsequent construction of the C/D rings with tryptamine completed the synthesis of yohimbine. However, these conventional approaches required relatively lengthy synthetic sequences to control stereochemistry and to make pentacyclic structure. In this poster presentation, our endeavor towards the development of a new synthetic approach for yohimbine will be presented. The cyanide-catalyzed imino-Stetter reaction of aldimine derived from 2-aminocinnamic acid derivative and pyridine-2-carboxaldehyde bearing acetyl group at the C5-postionprovided the corresponding indole-3-acetic acid derivative. Subsequent formation of the 6-membered C-ring followed by Michael addition of the malonate at C-15 position provided a rapid access to the pentacyclic intermediate. By controlling the stereochemistry after next several steps, it is expected that synthesis of yohimbine alkaloids could be completed.

Poster Presentation : **ORGN.P-627**
Organic Chemistry
Event Hall FRI 11:00~13:00

Asymmetric Total Syntheses of 7,8’-Coupled Naphthylisoquinoline Alkaloids via Atroposelective reduction

Taelyn Kim, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Naphthylisoquinoline alkaloids have attracted considerable attention from the chemical community because of their unprecedented structural diversities and promising biological activities. Especially, 7,8’-coupled natural products exhibit interesting biological activities, such as antimalarial, antiplasmodial, antiparasitic and antitrypanosomal activities. However, because these natural products possess both central and axial chiralities, they have been considered synthetically challenging targets. Although 7,8’-coupled naphthylisoquinoline alkaloids consist of one of the main subclasses of these alkaloids, synthetic routes for accessing 7,8’-coupled naphthylisoquinoline alkaloids have been poorly explored; only one example of the total synthesis of 7,8’-coupled naphthylisoquinoline alkaloid without no axial chirality was reported to date. Furthermore, no attempts to control atroposelectivity in the 7,8’-coupled naphthylisoquinoline alkaloids has been made so far. Recently, our group reported the total syntheses of naphthylisoquinoline alkaloids via atroposelective coupling reaction using the internal central chirality at the C-3 position of the isoquinoline ring as the atroposelectivity-controlling group.1,2 As our continuing efforts on the atroposelective total syntheses of naphthylisoquinoline alkaloids, we investigated the atropselective synthesis of 7,8'-coupled naphthylisoquinoline alkaloids using the internal central chirality in the isoquinoline ring as an atroposelectivity-controlling group. In this poster presentation, we will describe the asymmetric total syntheses of several 7,8'-coupled naphthylisoquinoline alkaloids.Reference1.Kim, K.-H.; Cheon, C.-H. Advanced Synthesis & Catalysis, 2016, 358, 2883-2888 2.4. Kim, K.-H.; Cheon, C.-H. Organic Chemistry Frontiers, 2017, 4, 1341-1349.3.Jo, Y.-I.; Lee, C.-Y.; Cheon, C.-H. Org. Lett. 2020, 22, 4653.4.Jo, Y.-I.; Lee, C.-Y.; Cheon, C.-H. J. Org. Chem. 2020, 85, 12770.

Poster Presentation : **ORGN.P-628**
Organic Chemistry
Event Hall FRI 11:00~13:00

Total Synthesis of Rucaparib

Ju-Ahn Seo, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Rucaparib is a poly(ADP-ribose) polymerase (PARP) inhibitor used as an anti-cancer agent. It received an approval by the Food and Drug Administration (FDA) for the treatment of ovarian and prostate cancer in 2016 and 2020, respectively. Structurally, rucaparib possesses an indole subunit bearing four substituents along its periphery and an additional seven-membered lactam ring between the two substituents at C3 and C4 positions. As an indole derivative bearing the four desired substituents at appropriate positions is not readily available, most of the previous syntheses have been developed based on the protocol for the preparation of the tetra-substituted indole derivatives. Recently, our group developed a highly efficient protocol to access 2-substituted indole-3-actetic acid derivatives via the cyanide-catalyzed imino-Stetter reaction of aldimines obtained from 2-aminocinnamic acid derivatives and aldehydes. With this protocol in hand, we developed a new synthetic route for rucaparib. 2-Aminocinnamamide could be prepared from meta-fluorobenzoate, which currently used as the starting material in the process chemistry route of rucaparib, via benzylic olefination with glyoxalamide and subsequent reduction of the nitro group to amino group. The cyanide-catalyzed imino-Stetter reaction of aldimine, derived from the resulting 2-aminocinnamamide derivative and aldehyde, provided indole-3-acetamide bearing all three substituents at the right position. Final azepinone ring formation completed the total synthesis of rucaparib.

Poster Presentation : **ORGN.P-629**

Organic Chemistry

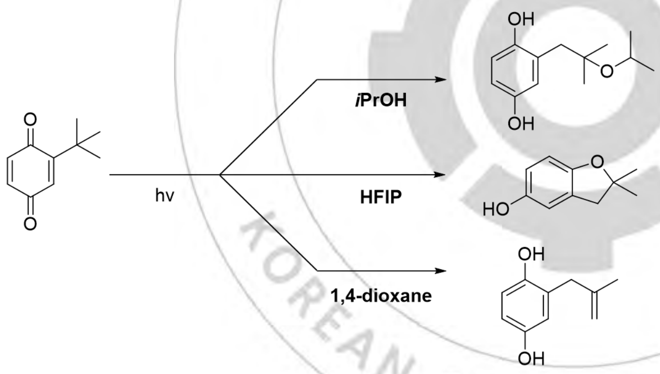
Event Hall FRI 11:00~13:00

Diverse C-H functionalization processes of 2-tert-butyl benzoquinones

<u>Cheol Hyeon Ka</u>, Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

Under photo-irradiation, benzoquinone is activated to its highly reactive triplet state. The photoexcited 2-tert-butyl benzoquinone can undergo facile 1,5-HAT (hydrogen atom transfer) process to afford diradical intermediate, which can be converted to the various compounds selectively dependant on solvent system.



Poster Presentation : **ORGN.P-630**

Organic Chemistry

Event Hall FRI 11:00~13:00

Phenothiazine-Based Hole Transport Materials for Perovskite Solar Cells

Keun Hyeong Park, Young S. Park*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Interfacial engineering has proven effective in enabling improvements in the performances in optoelectronic devices. In particular, self-assembled monolayer (SAM) as a hole selective contact has led to more than 21% in power conversion efficiency. Herein, we reported the synthesis and characterization of phenothiazine-based hole transport materials for inverted perovskite solar cell. In this study, we developed novel phenothiazine derivatives which have well aligned frontier molecular orbital energy levels for hole extraction and electron blocking. This material has shown improved the power conversion efficiency up to 22.4%.

Poster Presentation : **ORGN.P-631**
Organic Chemistry
Event Hall FRI 11:00~13:00

Synthesis and Characterization of Indolizine Derivatives for synergistic STING activation

Eunsu Kim, Hee Ra Jung[1], Eunha Kim[*], Sanghee Lee[2,*]

Department of Molecular Science and Technology, Ajou University, Korea
[1]*Creative Research Center for Brain Science, Korea Institute of Science and Technology, Korea*
[2]*Neuromedicin department, Korea Institute of Science and Technology, Korea*

STING (Stimulator of interferon genes), which switch tumor immunophenotype from ‘cold’ to ‘hot’ via stimulation of innate immunity, is attracted as next generation of cancer immunotherapy. Synthetic agonist or natural ligand that bind STING activate IFN-mediated immune responses, promote anti-cancer immunity, and signify promising preclinical outcome. However, ubiquitous STING expression result limit their application to a subset of tumors. Therefore, synergistic activator of STING pathway has been spotlighted. In this regard, we have confirmed that a specific indolizine derivatives is involved in STING pathway activation in previous study. Furthermore, we progress the characterization and synthesis of indolizine for cancer immunotherapy through synergistic STING activation. To find a more effective stimulator for STING activation and improve the immune modulation activity for STING-mediated immunotherapy, we conducted structure-activity relationship (SAR) study of indolizine scaffold. As a result, based on luciferase reporter gene assay, we confirmed a some indolizine compounds have the enhanced effect on activating STING pathway with the presence of cGAMP.

Poster Presentation : **ORGN.P-632**

Organic Chemistry

Event Hall FRI 11:00~13:00

Degradation of GFP protein with Hetero-bis-clickable linker platform for efficient PROTAC development

Eunsu Kim, JaeWan Kim[1], Jeonghyun Lee[2], Eunha Kim[*], Junwon Choi[3]

Department of Molecular Science and Technology, Ajou University, Korea
[1]*Molecular science & technology, Ajou University, Korea*
[2]*department of molecular science and technology, Ajou University, Korea*
[3]*Molecular Science and Technology, Ajou University, Korea*

PROTAC (proteolysis targeting chimera) is a heterobifunctional molecule made by the conjugation of two ligands (i.e., an E3 ligase ligand and a target protein ligand) with a chemical linker. PROTAC triggers the selective ubiquitination of the target protein, which leads removal of the protein of interest (POI). PROTAC technology is regarded as a promising platform that can provide a breakthrough for the bottleneck of drug discovery process. However, the discovery of optimized PROTAC is a labor-intensive and tedious process. Therefore, there is a huge demand for a platform technology to efficiently find optimal PROTAC for POI. To address unmet needs, here we represent proof of concept study for a PROTAC linker platform via utilization of SPAAC (Strain Promoted Azide-Alkyne Cycloaddition) and iEDDA (inverse-Electron Demand Diels-Alder reaction), which will be useful to study optimal linker length for diverse POIs. To minimize the perturbation of the original binding affinity of two different ligands, both POI and E3 ligase ligands were modified with azide and tetrazine. For a systematic study to evaluate the influence of the linker on the degradation efficiency of the target protein, a hetero-bis-clickable linker containing DBCO and TCO was constructed.

Poster Presentation : **ORGN.P-633**

Organic Chemistry

Event Hall FRI 11:00~13:00

One-Photon-Two-Electron Photoredoxcatalysis for Trifluoromethylation of Alkenes

Si Hyun Woo, Dayoon Song[1], Seunga Heo[1], Youngmin You[*]

Chemical Engineering and Materials Science, Ewha Womans University, Korea
[1]*Ewha Womans University, Korea*

Photoredoxcatalysis enables a variety of organic transformations under mild reaction conditions. However, photoredoxcatalysis developed thus far suffers low quantum yields because it enables one-electron transfer upon one-photon absorption. We hypothesized that singlet fission (SF), a process that generates two triplet excited states from one photon absorption, could double the quantum yield. To validate this hypothesis, we devised a phoredoxcatalytic trifluoromethylation protocol which employed 1,4-bis(6,11-bis(triisopropylsilylethynyl)tetracen-2-yl)benzene (Tet-Ph-Tet) as a SF photocatalyst, decamethylferrocene ($Me_{10}Fc$) as a sacrificial electron donor, and the Togni reagent as a $\bullet CF_3$ source. Photoirradiation (1.5 mW, green LEDs) of an Ar-saturated THF containing a 5-hexenol substrate, 1 mol % Tet-Ph-Tet, $Me_{10}Fc$, the Togni reagent, and potassium carbonate produced the desired 6,6,6-trifluoroheptanol. Our mechanistic studies indicated an occurrence of reductive electron transfer from Me10Fc to the correlated triplet excited-state Tet-Ph-Tet, to form a biradical dianion of Tet-Ph-Tet. This species can facilitate electron transfer to the Togni reagent. We hope that our research will be instrumental to substantially improve the efficiency of phororedoxcatalytic organic transformations.

Poster Presentation : **ORGN.P-634**

Organic Chemistry

Event Hall FRI 11:00~13:00

HEPES Repositioning: Disaggregating agent for Amyloid beta plaque and a new Sustained-release Formulation

Jaehoon Kim, Dokyoung Kim[1,*]

Department of Biomedical Science, Graduate School, Kyung Hee University, Korea
[1]*College of Medicine, Kyung Hee University, Korea*

Alzheimer’s disease (AD) is one of the degenerative brain diseases that occur with aging. As the aging society of mankind gradually deepens, it becomes a bigger social problem. In addition, since the exact cause of AD has not yet been found, treatment of the disease remains a serious problem. Here we introduced repositioning of HEPES (4-(2-hydroxyethyl)-1-piperazine ethane sulfonic acid). HEPES is a well-known buffer solution for material mainly used for cell culture because of its good effect of maintaining pH. However, in this study, we demonstrated a new efficacy for HEPES in disaggregating amyloid beta plaques, which are presumed to be the cause of AD. In this work, we proved that HEPES can disaggregate amyloid beta plaques using several probes capable of detecting amyloid beta plaques. These results showed better efficiency than EPPS ((4-(2-hydroxyethyl)-1-piperazine ethane sulfonic acid), which was previously reported as a disaggregating agent of amyloid beta plaques. Furthermore, in order to improve the frequent drug intake, which is a very big disadvantage in Alzheimer's disease treatment, a drug release system that is released sustainably for about 2 weeks was introduced by hybridizing it with Eudragit S 100, a biocompatible polymer.

Poster Presentation : **ORGN.P-635**

Organic Chemistry

Event Hall FRI 11:00~13:00

Fluorescent Cysteine Probe: Cervical Cancer Diagnosis

Youngwoong Kim

Department of Biomedical Science, Kyung Hee University, Korea

Medical check-ups for the progress of cervical cancer that occurs in the cervix of females make the female feel reluctant because the medial check-up (Pap test) is performed by using a speculum into the vagina. Thus, diagnosis technology using biofluids such as plasma and urine is important to be convenient for the user. The in vitro fluorescent diagnostic probe using biofluids has been developed to be more precise and convenient for the user. Among biofluids, urine could clearly reflect their conditions when their biosystem has a disorder. Cysteine (Cys) is one of the thiol group-containing sulfur (-SH) in a biological system and has a potential of a biomarker for various diseases such as oxidative stress, Alzheimer's disease, and cancer. Herein, we disclose the new urinalysis to diagnose cervical cancer using fluorescent Cys probe (NPO-B). To be higher reliability and accuracy for diagnosis, the urine samples were carefully analyzed and obtained about 1,800 individuals with various diseases containing healthy control. Interestingly, NPO-B significantly reacted with cervical cancer while turning on the fluorescence. Based on this property, we verified the sensitivity and selectivity of NPO-B with Cys in urine using UV-Vis/fluorescence spectrophotometer. Additionally, urinalysis using NPO-B required a tiny amount of urine (200 □L) with a short diagnosis time (40 min). The synthesis of NPO-B was systemically verified by (1H and 19F) NMR and Mass spectrometer. Given the distinguished properties, our finding could become an alternative to the Pap test, which puts substantial physical and psychological burdens on the female. We also believe that our finding contributes to increasing the rate of diagnosis and health of females as well as proposing the future road for the field of the fluorescent diagnostic probe.

Poster Presentation : **ORGN.P-636**

Organic Chemistry

Event Hall FRI 11:00~13:00

Controlling the screw sense of 12/10-helix β-Peptides by modifying terminal groups

Kyung In Jang, Soo Hyuk Choi[1,*]

Department of chemistry, Yonsei University, Korea
[1]*Department of Chemistry, Yonsei University, Korea*

Peptide oligomers with specific β-amino acids adopt 12/10-helical structure. Especially, cis-2-aminocyclohexanecarboxylic acid (cis-ACHC) is a well-known cyclic β-amino acid which forms 12/10-helix structure. Heterogeneous cis-ACHC oligomers with alternating chirality show rapid interconversion between two conformations, P-helix (right-handed) and M-helix (left-handed) in solution. Our main focus is on controlling this relative population by introducing functional group at the N-terminal in oligomer. We introduced several functional groups that might prefer a specific screw sense. Our group synthesized various tetrapeptides that have different terminal group. To specify helical screw sense tendency, circular dichroism analysis was conducted under protic and aprotic solvents. Effects of terminal group modification are also indicated by single crystal X-ray diffraction.

Poster Presentation : **ORGN.P-637**

Organic Chemistry

Event Hall FRI 11:00~13:00

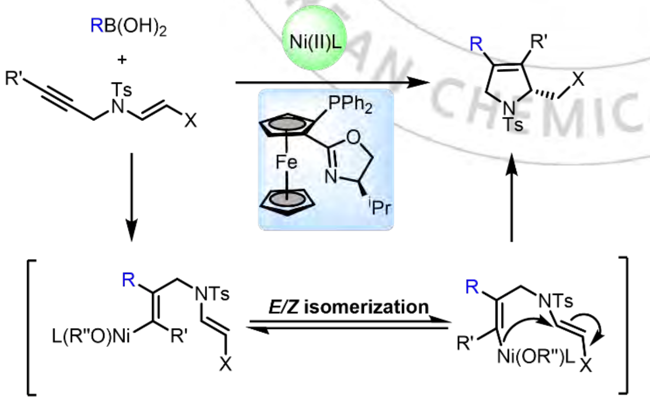
Ni-Catalyzed Enantioselective Synthesis of 2,3,4-trisubstituted 3-pyrrolines

Shrikant Tambe, Eun Jin Cho[1,*]

Department of chemistry, Chung-Ang University, India

[1]*Department of Chemistry, Chung-Ang University, Korea*

The development of synthetic methods for highly functionalized chiral 3-pyrrolines is a valuable venture due to the prevalence in natural and synthetic bioactive molecules. Unfortunately, the previous general cycloaddition approaches using allenes cannot provide 3,4-disubstituted 3-pyrrolines. Herein, an unconventional approach yielding 2,3,4-trisubstituted 3-pyrrolines with a chirality at 2-position is presented. A simple catalytic system of Ni(II)/Fc- *i*-PrPhox facilitates the highly stereoselective process to give enantioselectivity up to 99%. The enantioenriched 3-pyrrolines can be converted into other attractive classes of N-heterocycles.



- enantio/regio selective
- amino acrylic system as an electrophile
- 3,4-biaryl substituted 3-pyrrolines
- easily synthesized SM
- product manipulation

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Poster Presentation : **ORGN.P-638**
Organic Chemistry
Event Hall FRI 11:00~13:00

Conformational analysis of β-peptides containing *trans*-4,4-dimethyl-2-aminocyclopentanecarboxylic acid (*trans*-dmACPC)

Heewon Choi, Soo Hyuk Choi[1,*]

chemistry, Yonsei University, Korea
[1]*Department of Chemistry, Yonsei University, Korea*

Peptide foldamers can display a specific secondary structure by different hydrogen bonding patterns. It is well known that *trans*-2-aminocyclopentanecarboxylic acid (*trans*-ACPC) oligomers adopt 12-helical conformations. By replacing *trans*-ACPC with *trans*s-dmACPC, an unusual secondary structure can be formed. A previous work suggests that oligomers of *trans*-dmACPC and *trans*-ACPC show distinctive nuclear Overhauser effects (NOEs) that implies 16-helix structure. Our group synthesized oligomers that consist of *trans*-ACPC and *trans*-dmACPC. Conformational analysis was conducted through Circular Dichroism and NMR methods.

Poster Presentation : **ORGN.P-639**

Organic Chemistry

Event Hall FRI 11:00~13:00

Conformation of Valine-based D,L-peptides containing β-amino acids

Eunjin Seo, Soo Hyuk Choi[1,*]

Department of chemistry, Yonsei University, Korea

[1]*Department of Chemistry, Yonsei University, Korea*

D,L-peptides are natural peptides with alternative L- and D- amino acids. Gramicidin and Feglymycin are naturally occurring D,L-peptides which are representatives of carrier and channel-type ionophores. Gramicidin A is known to form various β-helix structures on different environment. Conformation of Boc- and MeO- protected D,L- oligopeptides derived from Valine have been previously studied. In particular, Boc-(L-Val-D-Val)4-OMe is known to form double-stranded β-helical dimers with antiparallel chains. We synthesized D,L-hepta,-octapeptdes that contain a few β-amino acids to mimic valine based D,L-oligopeptide. We introduced (1S,2R)-cis-2-aminocyclohexane carboxylic acid (cis-ACHC) to control helical structure. We analyzed conformations of D,L-peptide by NMR, CD and X-ray crystallography.

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Poster Presentation : **ORGN.P-640**

Organic Chemistry

Event Hall FRI 11:00~13:00

C-H bond functionalization reaction by Ag/Pd multimetallic active catalyst: Computational study on mechanism

Taebin Jung, Youn Kyung Kang*, Ji Eun Park[1]

Department of Chemistry, Sangmyung University, Korea
[1]*Department of Chemistry, Seoul National University, Korea*

The mechanism of 2-arylation of benzofuran by Ag/Pd multimetallic catalyst system has been examined by using DFT (wb97xd) computational methods. A number of different catalyst systems that include $[Pd(OAc)_2]$, $[Pd(OAc)_3]^-$, $[Pd(OAc)_2(OH)]^-$, $[Pd(OAc)_2(Ph)]^+$, $[Pd(OAc)_3(Ph)]$, $[Pd(OAc)_2(OH)(Ph)]$, $[PdAg(OAc)_2]$ were considered as active catalyst species. The lowest-energy pathway involves an oxidative addition by Ag(I)-Pd(II) multimetallic active catalyst species/carboxylate-assisted-C(sp2)-H activation by Pd(IV) active catalyst species featuring a Wheland intermediate/reductive coupling cycle. The rate determining step was found to be the oxidative addition, which has energetic span of 19.6 kcal/mol. The C(sp2)-H activation was followed by the Pd(IV) catalyst species after forming a Wheland intermediate which has long been recognized as the manifestation for the electrophilic aromatic substitution (SEAr) mechanism yet never been identified computationally. Based on this pathway, the detailed role of Ag additives was elucidated.

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Poster Presentation : **MEDI.P-359**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery of indolin-2-one analogs as PIM kinase inhibitors

Hyeonseong Choo, Jinho Lee*, Victor Sukbong Hong*

Department of Chemistry, Keimyung University, Korea

Proviral Integration Moloney murine leukemia virus (PIM) kinase, which is involved in the regulation of cellular processes such as survival, proliferation, cell cycle regulation, is overexpressed in hematological and solid cancers. It is a serine/threonine kinase with three homologous isomers of PIM-1, PIM-2, and PIM-3. PIM-1 kinase characteristically has a proline residue (Pro123) in the hinge region of the ATP binding site, and show high selectivity over other kinase inhibitors.In this study, using an indolin-2-one scaffold a series of novel compounds were designed and synthesized for PIM kinase inhibitor. Multiple substituents were introduced to the scaffold to make effective interaction not only with the carboxyl groups of Asp128 and Glu121, but also with the amino group of Lys67 of PIM-1 kinase. As a result of structure-activity relationship (SAR) study, the most potent inhibitor yielded IC_{50} values of 5.6 nM and 6.9 nM for PIM-1 and PIM-3, respectively.

Poster Presentation : **MEDI.P-360**

Medicinal Chemistry

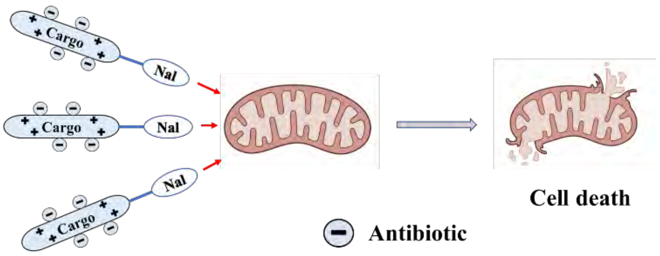
Event Hall THU 11:00~13:00

Improved mitochondria-targeting, lipophilicity, and drug delivery using guanidine moieties

Akula Murthy, Jungkyun Im*

Department of Electronic Materials and Devices Engineering, Soonchunhyang University, Korea

Mitochondria are responsible for carrying multiple cellular functions from energy production to cell apoptosis. On other hand, the dysfunction of mitochondria is directly associated with diverse human diseases. Directing therapeutic agents to mitochondria provide new approaches for disease treatment. Although many strategies have been developed to target mitochondria, efficient delivery to mitochondria is still a hot pot in clinical applications. Evidences are suggesting that guanidines are prevalent in targeting mitochondria. Based on our search for efficient subcellular localization, a sorbitol-based molecular transporter having guanidines was prepared. Further, the lipophilic nature of the transporter was improved by attaching alanine-naphthalene to facilitate the penetration through the cell- and mitochondrial membranes. Charges of the transporter and the antibiotics supported the strong interactions to form an ionic bonding between them. Cell viability test was demonstrated that the transporter itself favorable to delivering drugs to mitochondria. In-depth investigations were carried out in in-vitro studies for elucidating the efficiency of the transporter in mitochondrial targeting. The results from investigations demonstrated the efficient delivery and have gained much interest in selective strategies toward mitochondria.



Poster Presentation : **MEDI.P-361**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Photodynamic Therapy OFF/ON System-Based Stimuli-Responsive Multi-Cancer Therapy

Huiqiang Wu, Il Yoon*

Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea

The development of cancer therapy based on non-invasive and patient friendly — Photodynamic Therapy (PDT) has attracted extensive attention. It is to develop a cancer treatment without side effects through the synergy of PDT/ photothermotherapy (PTT)/Chemo. Using nanoparticles to synthesize high concentration photosensitizer (PS) is an effective method. To achieve this research target, a dimeric structure of pyropheophorbide-a derivative was proposed, this study was achieveable through designing and synthesizing the dimer structure of PS. The dimeric structure consists of two pyropheophorbide-a molecules that can efficiently inhibit generation of singlet oxygen ($^1O_2$) by providing a very close distance (Self-quenching).Therefore, for the dimeric PS, the length, flexibility and rigidity of the linker between the two pyropheophorbide-a molecules are vital to be used to facilitate the rational design of activatable photosensitizers.

Poster Presentation : **MEDI.P-362**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Structure-Based Virtual Screening: Identification of a Novel NS2B-NS3 Protease Inhibitor with Potent Antiviral Activity against Zika and Dengue Viruses

Joo-Youn Lee

Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea

Zika virus (ZIKV), which is associated with severe diseases in humans, has spread rapidly and globally since its emergence. ZIKV and dengue virus (DENV) are closely related, and antibodydependent enhancement (ADE) of infection between cocirculating ZIKV and DENV may exacerbate disease. Despite these serious threats, there are currently no approved antiviral drugs against ZIKV and DENV. The NS2B-NS3 viral protease is an attractive antiviral target because it plays a pivotal role in polyprotein cleavage, which is required for viral replication. Thus, we sought to identify novel inhibitors of the NS2B-NS3 protease. To that aim, we performed structure-based virtual screening using 467,000 structurally diverse chemical compounds. Then, a fluorescencebased protease inhibition assay was used to test whether the selected candidates inhibited ZIKV protease activity. Among the 123 candidate inhibitors selected from virtual screening, compound 1 significantly inhibited ZIKV NS2B-NS3 protease activity in vitro. In addition, compound 1 effectively inhibited ZIKV and DENV infection of human cells. Molecular docking analysis suggested that compound 1 binds to the NS2B-NS3 protease of ZIKV and DENV. Thus, compound 1 could be used as a new therapeutic option for the development of more potent antiviral drugs against both ZIKV and DENV, reducing the risks of ADE.

Poster Presentation : **MEDI.P-363**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Fluorescence Intensity techniques for discovery and characterization of protein tyrosine phosphatase SHP2 inhibitors

Jihoon Park

Chemistry, Keimyung University, Korea

Scr homology region 2-containing protein tyrosine phosphatase 2 (SHP2) is a non-receptor protein tyrosine phosphatase encoded by *ptpn11gene*. SHP2 plays an important role in cell signaling pathways involved in cell growth, death, DNA damage, DNA replication, and drug resistance. SHP2 has been studied as a promising anticancer target because it is overexpressed in various cancers such as breast cancer, lung cancer, and laryngeal cancer. We identified novel SHP2 inhibitors, compound (**1**) and compound (**2**) using a sensitive fluorescence intensity assay optimized in 384-well plate format. Kinetic studies revealed that both compound (**1**) and compound (**2**) showed noncompetitive mechanism of inhibition with K_i values of 1.2 nM and 1.5 nM against DiFMUP substrate, respectively, indicating they may be allosteric inhibitors. The dissociation rate constants of the compounds were measured using the jump dilution method. It was concluded that both compound (**1**) and compound (**2**) are potent and slowly reversible inhibitors of SHP2. In addition, the results of the IC_{50} shift assay indicated that compound (**1**) and compound (**2**) caused time-dependent inhibition with a 10-fold and a 9-fold change in IC_{50} during incubation, respectively.

Poster Presentation : **MEDI.P-364**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Identification and characterization of menin-MLL1 interaction inhibitor by small-molecule library screening with a TR-FRET based assay

Yeonwoo Kim

College of Natural Sciences/Chemistry, Keimyung University, Korea

Menin protein encoded by the *MEN1* (multiple endocrine neoplasia type 1) gene is involved in epigenetic processes and gene transcriptional regulation via interaction with protein partners in chromatin-associated protein complexes and transcription factors. The interaction between the menin and the histone methyltransferase MLL1 (mixed-lineage leukemia 1) is critical for development of human acute leukemia. Therefore, inhibition of the menin-MLL1 interaction with small molecules would be a useful approach to develop new anticancer agents. We have developed a high-throughput assay in a 384-well format using time-resolved fluorescence resonance energy transfer (TR-FRET) to identify small molecules that inhibit the menin-MLL1 interaction. We screened a small-molecule library of 160 compounds at 10 μM compound concentration and identified one validated hit with an IC_{50} value of 1.1 μM. We further evaluated the ability of the hit compound to reduce MV4-11 cell viability by performing fluorescence-activated cell sorting (FACS) analysis.

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Poster Presentation : **MEDI.P-365**
Medicinal Chemistry
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MPO-0063 as a mPGES-1 inhibitor alleviated the symptoms of acute brain ischemia in mice models

Seyoung Yang, Gwon Minju, Minji Kim, Hyemin Choi, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

The accumulation of prostaglandin E2 (PGE$_2$) has been demonstrated at the lesion sites of rodent ischemia models. It was recently identified that both microsomal prostaglandin E synthase-1 (mPGES-1) and cyclooxygenase-2 (COX-2), key enzymes for PGE$_2$ biosynthesis, were observed after brain ischemia. In addition, many evidences suggest that mPGES-1 and COX-2 are co-induced by excessive glutamate in the ischemic brain and act together to exacerbate stroke injury through PGE$_2$ production followed by activation of EP3 receptors. In order to investigate therapeutic effects of mPGES-1 inhibitor on ischemic excitotoxicity, therefore, our lead compound **MPO-0063** was evaluated using mice brain ischemia models. As a result, systemic treatment with **MPO-0063** (5 or 10 mg/kg, i.p.) after transient middle cerebral artery occlusion (MCAO) improved post-stroke well-being, decreased infarction and edema, suppressed induction of brain cytokines, alleviated locomotor dysfunction and anxiety-like behavior, and reduced the long-term cognitive impairments. These overall experimental results suggest that mPGES-1 inhibitor could be used as a therapeutic agent for ischemic stroke.

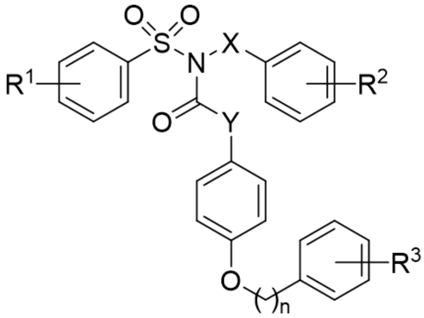
Poster Presentation : **MEDI.P-366**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Synthesis and structure-PGE$_2$ production inhibitory relationship of phenylsulfonamide derivatives

Jiwon Woo, Seyoung Yang, Gwang Hyun Moon, Junseong Ahn, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

The inhibition of prostaglandin E$_2$ (PGE$_2$) production is an important target of anti-inflammatory drugs. Microsomal prostaglandin E synthase-1 (mPGES-1) is responsible for the massive PGE$_2$ formation during inflammation. Many evidences reveal mPGES-1 inhibitors as a safe alternative to nonsteroidal anti-inflammatory drugs (NSAIDs) and cyclooxygenase-2 (COX-2). For the discovery of novel mPGES-1 inhibitors, a series of phenylsulfonamide derivatives was synthesized and screened for their *in vitro* inhibitory effects on PGE$_2$ production from RAW 264.7 macrophage cells and A549 human cancer cells induced by LPS and IL-1β, respectively. Structure–activity relationship study suggested that inhibitory activity of synthetic derivatives against PGE$_2$ formation was governed to a greater extent by the substituent R^1 and/or R^2, and more importantly, their metabolic stabilities were found to be dependent on the characteristic (X or Y) of N-substituent. The relationship between phenylsulfonamide structures and their PGE$_2$ inhibitory activities was also interpreted by both mPGES-1 assay and molecular docking study on mPGES-1.



X = NH, CH$_2$
Y = O, NH
n = 1, 4

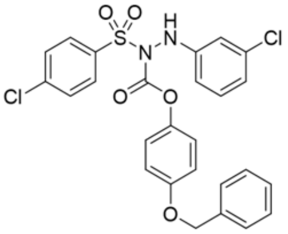
Poster Presentation : **MEDI.P-367**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Characterization of MPO-0144 as a novel mPGES-1 inhibitor in the adjuvant-induced arthritis (AIA) rodent models

Gwang hyun Moon, Seyoung Yang, Junseong Ahn, Jiwon Woo, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

Prostaglandin E_2 (PGE_2) production is an important target of anti-inflammatory drugs. PGE_2 is produced upon the conversion from arachidonic acid into prostaglandin H_2 (PGH_2) by cyclooxygenase-1 (COX-1) and COX-2, and subsequent conversion from PGH_2 to PGE_2 by three isoforms of prostaglandin E synthase (PGES): cytosolic PGES (cPGES), microsomal PGES-1 (mPGES-1), and mPGES-2. There is an established fact that both inducible enzymes COX-2 and mPGES-1 are responsible for the inflammatory PGE_2 production. Therefore, mPGES-1 is a more promising ideal target for anti-inflammatory drugs. As our continuous research for the discovery of novel mPGES-1 inhibitors, herein, we characterized **MPO-0144** as a mPGES-1 inhibitor and evaluated its anti-inflammatory effects using in vivo experimental models. **MPO-0144** strongly inhibited LPS-induced PGE_2 production (IC_{50} = 41.8 nM) in RAW 264.7 cells via the inhibition of murine mPGES-1 activity (IC_{50} = 1.16 nM) together with selectivity over COX-1/2. A molecular docking study theoretically suggests that **MPO-0144** could inhibit PGE_2 production by blocking the PGH_2 binding site of mPGES-1 enzyme. In adjuvant-induced arthritis (AIA) rodent models, **MPO-0144** significantly diminished the paw edema without gastric inflammation and liver, kidney, heart toxicities. Thus, our data suggest that **MPO-0144** downregulates PGE_2 production by interfering with the mPGES-1 activity, thus reducing edema in AIA rodent models.



MPO-0144

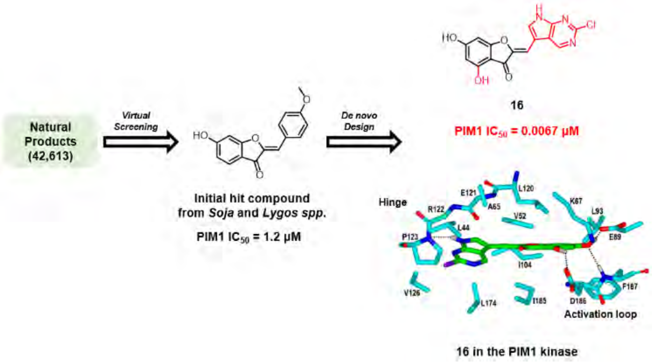
Poster Presentation : **MEDI.P-368**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery of PIM1 Inhibitor with Anticancer Activity from Structure-Based Virtual Screening of Natural Products.

Kewon Kim, Sungwoo Hong*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The proviral insertion of Moloney Murine leukemia (PIM) 1 kinase has gained attention due to its crucial role in enhancement of cell proliferation and the inhibition of apoptosis. To discover promising PIM1 kinase inhibitors, structure-based virtual screening of natural products of plant origin and de novo design were carried out using the protein-ligand binding free energy function improved by introducing an adequate dehydration energy term. As a result of subsequent enzyme inhibition assays, four classes of PIM1 kinase inhibitors were discovered, with the biochemical potency ranging from low-micromolar to sub-micromolar levels. The results of extensive docking simulations showed that the inhibitory activity stemmed from the formation of multiple hydrogen bonds in the combination with hydrophobic interactions in the ATP-binding site. Optimization of the biochemical potency by chemical modifications of the 2-benzylidenebenzofuran-3(2H)-one scaffold led to the discovery of several nanomolar inhibitors with antiproliferative activities against human breast cancer cell lines. These new PIM1 kinase inhibitors are anticipated to serve as a new starting point for the development of cancer treatment.



Poster Presentation : **MEDI.P-369**

Medicinal Chemistry

Event Hall THU 11:00~13:00

LCK/FMS dual inhibitors based on phenoxypyrimidine scaffold as candidate compounds for antiinflammatory disorders

So Jin Kang, Yongseok Choi, Eun Joo Roh[1,*]

Department of Biotechnology, Korea University, Korea

[1]*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

The aim of this study is to design and synthesize new pyrimidine-based molecules with phenoxypyrimidine scaffolds able to inhibit Tyrosine kinase including LCK and FMS. For this study, 32 imine, 11 amine and 2 benzamide derivatives bearing an phenoxypyrimidine scaffold were designed, synthesized, and biologically evaluated against LCK and FMS. The most active LCK derivative was **8b** with an IC_{50} 101nM, introducing it as a initial hit for further modifications for inflammation-associated disease. Compound **9k** showed excellent inhibition values with an IC_{50} 3.0nM. There are also compounds activated in both LCK and FMS. Compound **9c** is imine derivative with an IC_{50} value 1640 and 14.9nm respectively. Compound **12c** is amine derivative with an % Enzyme inhibition value 99.37% and 96.86% respectively. Compound **13b** is benzamide derivative with an % Enzyme inhibition value 97.39% and 95.38% respectively.

Poster Presentation : **MEDI.P-370**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis and Biological Evaluation of 2-Benzylaminoquinazolin-4(3H)-ones Derivatives as a Potential Treatment for SARS-CoV-2

Jun Young Lee, Chul Min Park[1,*]

CEVI, Korea Research Institute of Chemical Technology, Korea
[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Despite the continuing global crisis caused by COVID-19, there is still no effective treatment. Therefore, we designed and synthesized a novel series of 2-benzylaminoquinazolin-4(3H)-one derivatives and demonstrated that they are effective against SARS-CoV-2. Among the synthesized derivatives, 7-chloro-2-(((4-chlorophenyl)(phenyl)methyl)amino)quinazolin-4(3H)-one (lead compound) showed highest anti-SARS-CoV-2 activity, with a half-maximal inhibitory concentration value greater than that of remdesivir (IC50 = 4.2 μM versus 7.6 μM, respectively), which gained urgent approval from the FDA. In addition, our lead compound showed good results in various assays measuring metabolic stability, hERG (human ether a-go-go), CYP inhibition, and PPB, and showed better solubility and pharmacokinetics than our previous work.

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Poster Presentation : **MEDI.P-371**

Medicinal Chemistry

Event Hall THU 11:00~13:00

N-(Biphenyl-3-ylmethyl)ethanamines as G protein-biased agonists of 5-HT$_7$R

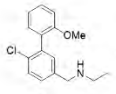
Hyunji Oh, Yeonji Oh[1], Jihye Seong[2], Byungsun Jeon[1], Jaekyun Lee[1], Bongjin Moon, Taek Kang[1,*], Hyunah Choo[1,*]

Department of Chemistry, Sogang University, Korea

[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

[2]*Center for Neuromedicine, Korea Institute of Science and Technology, Korea*

There has been much attention to biased ligands of G protein-coupled receptors (GPCRs) for potential pharmacological benefits. Recently, we reported N-((6-chloro-2'-methoxy-[1,1'-biphenyl]-3-yl)methyl)ethanamine **1** as G protein-biased agonist of 5-HT$_7$R, which could be used as a chemical probe for study on treatment discovery of autism spectrum disorder. Herein, we describe the synthesis of derivatives of the compound **1** and their biological evaluations in both G protein and β-arrestin signaling pathway. Total 16 compounds were synthesized and evaluated, and the compounds **7c**, **7f**, **7i**, and **7p** could be called as G protein-biased agonists like the compound **1**. Among the four compounds, the compound **7c** was the best in efficacy with an E_{max} value of 73% and the compound **7f** was the most potent agonist with an EC_{50} value of 0.094 μM.



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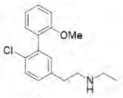

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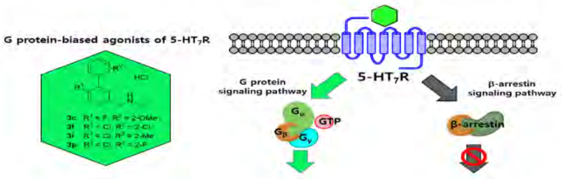

Poster Presentation : **MEDI.P-372**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery of 5-HT$_7$R Ligands Activating the G$_{12}$ Signaling Pathway

Diana Avramets, Jeong Hyun Jeong, Hyunah Choo*

Brain Science Institute, Korea Institute of Science and Technology, Korea

In regards to the recent findings, 5-HT$_7$R was demonstrated as a key player in memory, learning, cognitive functions, and other neurological processes. The coupling with the different downstream effectors which include the G$_S$-cAMP-dependent pathway, β-arrestin, and G$_{12}$-Rho-GTPases has already proved its impact on neurite growth and synaptic plasticity modulation in several studies. Here we hypothesized that screening for the biased ligands which activate the G$_{12}$ protein and, subsequently, related signaling network may become a plausible target for the drug development for the autism spectrum disorder (ASD) because the deteriorated neuritogenesis and synaptic network formation are well-known characteristics of the aforementioned disease. In this study, we screened more than 250 compounds library that included already developed nervous system receptors' ligands and approved drugs to identify 5-HT$_7$R agonists and antagonists biased specifically for downstream modulation of G$_{12}$ protein activity. We selected 13 compounds with antagonistic activity on the G$_{12}$-protein-mediated pathway for further dose-dependent cell-based luminescence assay to determine the most active compounds with their IC$_{50}$ values. Besides, the cell viability assay was performed to assess the toxicity of the chosen chemical compounds. Finally, the most active compounds were used for primary neuron culture treatment to estimate their effects on neurite growth.

Poster Presentation : **MEDI.P-373**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Photodynamic Therapy overcoming Tumor Hypoxia by Self-oxygen generation Catalase Conjugated Metal-Organic-Framework Nanosystem

Youjung Sim, Myoung Soo Lah[1,*], Ja-Hyoung Ryu[1,*]

Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Photodynamic Therapy (PDT) is a form of a phototherapy inducing cell death using light, oxygen and Photosensitizer (PS) which is generating ROS. These ROS interact with cellular components including lipids, amino acid and nucleic acids, and lead to the cell dysfunction. However, as a tumor grows, it rapidly outgrows its blood supply, leaving portions of the tumor where the oxygen concentration is significantly lower than in healthy tissues. For this reason, even effective photosensitizers cannot be working efficiently as much as expected. Therefore, if we overcome this hypoxia environment of tumor, photodynamic therapy can be more effective way forward. In our research, we conjugate the enzyme catalase (CAT) to surface of biocompatible nanocarrier MOF808. Catalase catalyzes the decomposition of hydrogen peroxide (H2O2) to water (H2O) and oxygen (O2). The generated oxygen can relieve the Hypoxia condition in tumor. Enriched oxygen further increases the PDT effect, enabling effective ROS generation. Also, immobilized enzyme is more stable than the free form of the enzyme enhancing the recyclability of enzymes and minimizing enzyme contamination.

Poster Presentation : **MEDI.P-374**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Drug delivery system of polymer-lipid hybrid nanoparticle formulation containing antisense oligonucleotide targeting ataxin-3

Jihyeon Lim

New Drug Discovery and Development, Chungnam National University, Korea

The main purpose of this study is to safely provide antisense oligonucleotides (ASOs) to ATXN3, the target gene of SCA3, through the development of polymer-lipid nanoparticles (PLNP). SCA3, a polyQ-derived disease, is directly induced by overexpression of the target protein, ATXN3. Therefore, regulating protein expression at the RNA level with ASOs allows for efficient treatment. However, it is easily degraded by endogenous nucleases, plasma proteins and has a fast half-life. And it is difficult to cross the limited space in the body like BBB. Therefore, overcome the limitations of ASOs by utilizing PLNP, which complemented the advantages of lipids and polymer carrier. Through compatibility experiments, DOTAP, lecithin, capryol90, and poloxamer were selected as lipids, solubilizers, and surfactants, respectively. PNLP was prepared using double solvent evaporation and centrifugation. The most reliable nanoparticles were formed when the L/P ratio was 1:7. As the content of poloxamer increased, nanoparticles with an encapsulation rate of 90% or more and delayed release of 35 days or more were secured. In particular, as the F127 content increased, the particle size became smaller, had a higher zeta potential, and the release was delayed. Through HeyA8 cells, intracellular delivery efficiency was significantly increased compared to the control group. However, it showed relatively low cell uptake efficiency. Therefore, the cell test was conducted by changing the sequence that can increase the cell uptake efficiency. In HEK293 cells, the level of target gene protein decreased as the ASO concentration of the formulation increased. In this way, PLNP helps to safely delivery ASOs to the target point. Therefore, PLNP is promising for RNA therapeutic drug delivery system.

Poster Presentation : **MEDI.P-375**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Keap1-modifying Small Molecule Ameliorates Parkinson’s Disease via Up-regulation of Antioxidants.

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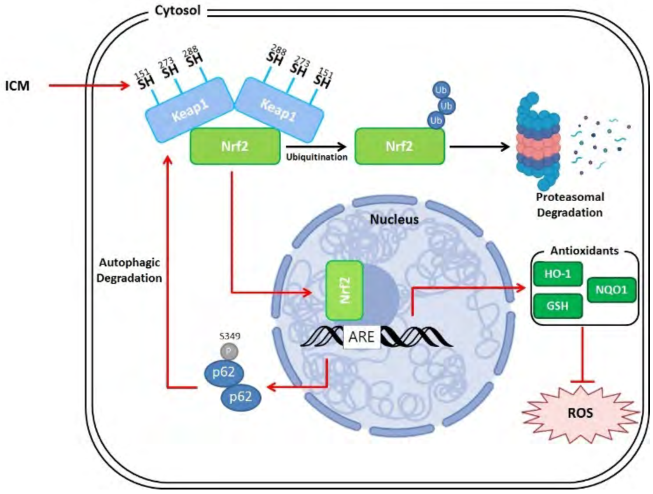
BioPhysics and Chemical Biology, Seoul National University, Korea

[1]*Division of Chemistry, Seoul National University, Korea*

Parkinson’s disease (PD) is the second most common neurodegenerative disease after Alzheimer’s disease. However, PD is a highly complex disease, and there is no adequate therapy except L-dopa treatment. We previously reported inflachromene (ICM) in our privileged Diversity-oriented synthesis (pDOS) library as a small-molecule modulator of neuroinflammation. We discovered that ICM could reduce mitochondrial dysfunction, one of the significant characteristics of PD, and protect neuronal cells from death in vitro and in vivo PD models.Our novel target ID method, Fluorescence difference in two-dimensional gel electrophoresis (FITGE), revealed that the target protein of ICM is keap1. ICM covalently bound to C151 of keap1 and liberated nrf2. Free-nrf2 translocated to the nucleus and increased p62 and various antioxidants, including NQO1, HO-1, and GSH. Up-regulated p62 and phospho-p62 (S349) induced autophagic degradation of keap1 in time-dependent manners, which resulted in the reinforcement of nrf2 with positive feedback. ICM ameliorated PD effectively via up-regulation of antioxidants. Collectively, our keap1-modifying small molecule can be effective therapeutics for PD. Since re-regulation of antioxidants is critical for treating neurodegenerative diseases, ICM may be good therapeutical candidates for other neurodegenerative diseases.


Cytosol
ICM
151 SH
273 SH
288 SH
Keap1
288 SH
273 SH
151 SH
Keap1
Nrf2
Ubiquitination
Ub
Ub
Ub
Nrf2
Proteasomal Degradation
Nucleus
Autophagic Degradation
Nrf2
ARE
Antioxidants
HO-1
NQO1
GSH
S349
P
p62
p62
ROS

Poster Presentation : **MEDI.P-376**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Plasmonic Nanostructure-based Light-enhanced Bioorthogonal Catalyst for Combinatorial Cancer Treatment

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Ewha Womans University, Korea
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The bioorthogonal reaction is any chemical reaction that can occur inside the living system without interfering with native biochemical processes. It can be a new powerful tool that facilitates the study of the structure and function of biomolecules and cellular manipulations within living systems. It can be widely used for imaging, detection, diagnostics, drug delivery, and biomaterials. Bioorthogonal catalysts could provide a platform for the changing of substrates to activated species that mimic the enzymes in biological reactions. Palladium catalysts are the highly efficient catalysts for the bioorthogonal reaction of prodrugs and pro-fluorophores, however, the intrinsically insufficient catalytic activities have restricted their biological in vivo application. Herein, we developed the palladium catalysts hybrid with plasmonic nanostructure to enhance the bioorthogonal catalytic activities by introducing light. The light can modulate the catalytic performance of these bioorthogonal nanocatalysts in terms of LSPR induced hot carrier generation and local field enhancement, which in return, would enhance the bioorthogonal catalytic activities and generate more activated drugs at the given condition. In addition, the photothermal effect will be incorporated to achieve synergistic photothermal and chemotherapy.

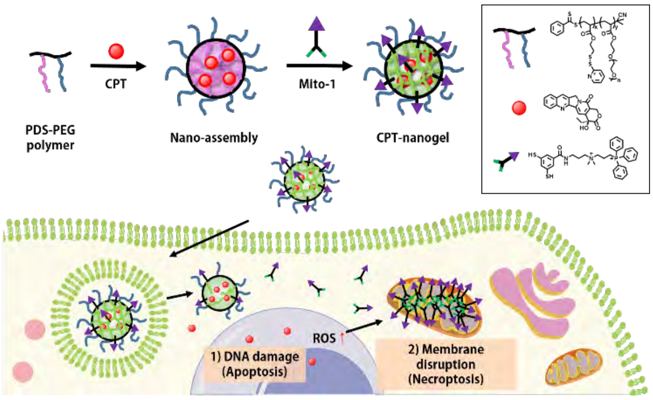
Poster Presentation : **MEDI.P-377**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Mitochondria-targeting self-assembly based on drug-loaded polymeric nanogel for combination therapy

Eun Seong Choi, Sangpil Kim[1], Ja-Hyoung Ryu*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Molecular Science, Ulsan National Institute of Science and Technology, Korea*

Mitochondria are important suborganelle that play a critical role in diverse cellular processes. Mitochondria-targeted therapeutic system has been emerged as potential novel strategy in cancer therapy. Mito-1, a small molecule containing triphenylphosphonium (TPP) and quaternary ammonium group, can target and accumulate in mitochondria due to its positive charge, leading to polymerization-induced self-assembly, PISA at high concentration in aconfined space. However, small molecule is exposed to biological environment before arrival at the desired tissue and cell. Herein, we designed mitochondria-targeting self-assembly derived from drug-loaded polymeric nanogel to maximize the therapeutic efficacy by combination therapy using anticancer drug, camptothecin (CPT), and self-assembly molecule, Mito-1. CPT loaded in the nanogel induces damage on nuclei DNA and apoptosis finally, while Mito-1 on the surface of nanogel as a crosslinker forms fibrous structure inside mitochondria which is large enough to disrupt the mitochondrial membrane, resulting necroptosis. By combined effect of apoptosis and necroptosis, nanogel system has shown cytotoxicity on HeLa cell and efficient mitochondrial membrane disruption was proved by mitochondria-related indicators.


PDS-PEG polymer
CPT
Nano-assembly
Mito-1
CPT-nanogel
ROS
1) DNA damage (Apoptosis)
2) Membrane disruption (Necroptosis)

Poster Presentation : **MEDI.P-378**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Preparation and characterization of docetaxel-loaded biocompatible multilayer nanoparticles

Jooyoung Ahn

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Docetaxel is known as an effective anticancer agent, but it is a poorly soluble drug that can result in low bioavailability. In this study, to solve this problem, the solubility was improved by polymeric micelle drug delivery system tri-block copolymer-based polymer known as a biocompatible polymer. In addition, for stabilization of micelles, liposomes were formed using lecithin, and micelles were encapsulated therein to prepare nanoparticles with a double-layered structure.The size of the docetaxel-encapsulated liposome nanoparticles was analyzed using ELS, and to confirm the double structure of nanoparticles, the cross-sectional structure was analyzed using cryo-TEM. In addition, an in vivo anticancer efficacy test against lung cancer cell line(A549) and breast cancer cell line(MDA-MB-2321) using a nude mouse was performed to compare the anticancer effect with a commercial docetaxel product (Taxotere) and an in vivo pharmacokinetic test using a rat was performed.Prepared DTX-LNPs showed the average particle size was 130±30 nm and maintained its size during stability test. As shown in Cryo-TEM image, it was confirmed that polymeric micelle nanoparticles were encapsulated inside the lecithin shell. In vivo anticancer efficacy test was conducted with prepared DTX-LNPs and Taxotere® into BALB/c nude mice transplanted with A549 and MDA-MB-231, and it was confirmed that the efficacy was significantly equivalent to that of the commercially used Taxotere®. Based on pharmacokinetic test results, it can be confirmed that the manufactured DTX-LNPs have a longer residence time in the body compared to Taxotere®, and the AUC and Cmax are significantly higher, indicating that the bioavailability is improved.

Poster Presentation : **MEDI.P-379**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery and synthesis of novel WRN helicase inhibitors for treating cancers with microsatellite instability

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[1]*Department of Chemistry, Korea Institute of Science and Technology, Korea*
[2]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

Microsatellite instability (MSI) refers to the condition which is genetically hyper-mutable due to defect in DNA mismatch repair system. MSI is reported as a key biomarker in colorectal, endometrial, gastric and ovarian cancers. From a therapeutical point of view, inhibition of DNA helicases can target DNA repair pathways in MSI cancer which induce synthetic lethality that promoting apoptosis and cell cycle arrest. In this work, we discovered small molecule inhibitors targeting Werner syndrome helicase (WRN helicase), one of the RecQ family DNA helicases. We ran a virtual screening on 1,678 ligands via docking study and sorted out the 6 structurally-diverse hit compounds. We identified TK-WRN-4 as a potent WRN helicase inhibitor through cell study on human colon cancer cell (HCT116) and confirmed the binding to WRN with thermal shift assay and cellular thermal shift assay. Then we synthesized TK-WRN-4 derivatives for optimization and finally discovered TK-WRN-22 as a new small molecule WRN inhibitor.

Poster Presentation : **MEDI.P-380**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Hyaluronic Acid – Based ROS – Responsive Micelles for Cancer Treatment

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[1]*chemistry, Ulsan National Institute of Science and Technology, Kazakhstan*

To date, chemotherapy is the main weapon against the last stages of cancer. Despite indisputable advances in science and technology over the last hundreds of years, chemotherapy still has number of drawbacks and limitations. High toxicity and solubility issues of the chemotherapeutic drug in pair of low delivery efficiency leads to severe side effects and rapid clearance. Therefore, it is important to design a potent carrier for precise and effective drug delivery. Recently, Hyaluronic acid polysaccharide–based drug conjugates have gained mass of attention due to their “stealth” effect that hides the nano system from protein corona formation. Moreover, the backbone of the polymer can be modified with chemotherapeutic through microenvironment–controlled linker. In this work, Camptothecin (CPT) anticancer drug was covalently bind to a Hyaluronic acid (HA) by Thioketal ROS–responsive linker (TK) to form amphiphilic prodrug (HTC). Hyaluronic acid is well known as biocompatible and biodegradable material used in cosmetic and medical spheres, that can also play a role as a drug carrier with active targeting for CD44 glycoprotein that is overexpressed in several cancer cell types. In this study, we designed and synthesized stimuli–responsive polymer–drug conjugates for improved targeting of cancer cells which self–assemble into core/shell micelles in aqueous media. The system will safely deliver the drug due to covalent binding and target CD44 receptor. The micelles will degrade under hyaluronidase and release the drug specifically on the tumor site under high ROS level.

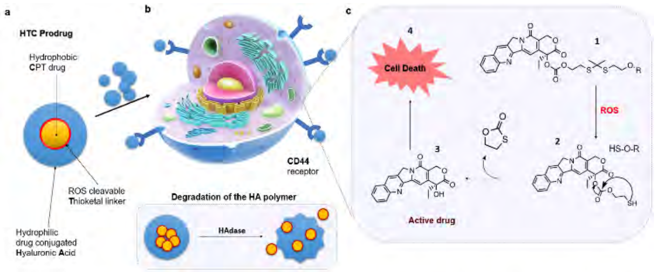

Figure 1. Schematic representation of CPT conjugated hyaluronic acid-based prodrug. **a)** schematic micelle structure of HTC prodrug. **b)** CD44 receptor induced targeting and endocytosis. Degradation of the Hyaluronic acid in TME. **c)** ROS triggered thioketal linker cleavage mechanism. Numbers shows an order of the process.

Poster Presentation : **MEDI.P-381**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery of Novel Phosphopantetheinyl Transferase Inhibitors Against Mycobacterium Tuberculosis

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[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*
[2]*Beamline Department, PAL-XFEL, Korea*

Tuberculosis (TB) is a potentially serious infectious disease usually caused by *Mycobacterium tuberculosis* (Mtb) bacteria that mainly affects the lungs, but could also affect other parts of the human body. TB is spread from person to person through the air. When people with lung TB cough, sneeze or spit, they propel the TB germs into the air. A person needs to inhale only a few of these germs to become infected. About one-quarter of the world's population has a TB infection, which means people have been infected by TB bacteria but are not (yet) ill with the disease and cannot transmit it. Treatment of TB uses antibiotics to kill the bacteria. Effective TB treatment is difficult, due to the unusual structure and chemical composition of the mycobacterial cell wall, which hinders the entry of drugs and makes many antibiotics ineffective. Therefore, blocking synthesis of lipids of Mtb’s cell wall has recently been attracting attention for the treatment of TB. Phosphopantetheinyl transferase (PptT), an enzyme that transfers 4′-phosphopantetheine (Ppt) from coenzyme A (CoA) to diverse acyl carrier proteins that synthesize the lipids critical to virulence as well as Mtb structural ingegrity. We discovered a hit via high throughput screening (HTS) and synthesized several compounds derived from it. Among them, two compounds showed good inhibitory activity in PptT more than the reference compound reported in Science. We are currently producing further modification of them that will be examined in the near future.

Poster Presentation : **MEDI.P-382**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Development of new drug candidates targeting angiotensin converting enzyme 2 and virus spike protein-protein interaction in SARS-CoV-2 infection

Dongwan Kang, Minwoo Kim[1], Seungik Jeong[1], Soong-Hyun Kim[1], Eunhye Lee[1], Yujin Park[1], Hyeongcheol Ham[1], Jee-Young Lee[2], Yuna Ha[2], Sejin Jung[1,*]

Medicinal chemistry, Korea Medical Develop Innovation hub, Korea
[1]*Department of Medicinal Chemistry, Korea Medical Develop Innovation hub, Korea*
[2]*Structure-based Drug Discovery, Molecular Design Team, Korea*

COVID-19 caused by severe acute respiratory syndrome coronavirus 2(SARS-CoV-2) was declared a pandemic in March 2020 and spread with unprecedented speed globally because of the continuous occurrence of variants. Interdisciplinary research is ongoing to develop vaccines and therapeutics to manage this infectious disease and numbers of vaccines are now commercially available. However, the effectiveness of vaccines against variants extremely dropped and this encourages the research of therapeutics for the treatment of COVID-19. The only FDA-approved orally administered antiviral treatment targeting SARS-CoV-2 is Paxlovid developed by Pfizer and it reduces the risk of hospitalization or death by 90%. However, it is necessary to develop a platform to treat COVID-19 efficiently due to its high cost and prescribing limitations caused by drug drug interactions. Therefore, we investigated the drug candidate against SARS-CoV-2.One of the potential drug targets is ACE2(angiotensin-converting enzyme 2) which induces the coronavirus into the host cell by recognizing the virus spike protein as host receptor and blocking the interaction between ACE2 and spike protein could lead to the prevention of SARS-CoV-2 infection. We have discovered compounds #15 and #34 as lead compounds obtained from *in silico* library screening combined with ACE2-RBD binding and *in vitro* antiviral assay. The results showed that compounds #15 and #34 prevent SARS-CoV-2 infection in Vero cell with IC_{50} values of 0.65 uM and 6.5 uM respectively, which are more potent or similar to the reference drugs, remdesivir and chloroquine in our assay system. In addition, ADME properties indicated that especially compound #15 is fairly stable in plasma and liver microsomes and has no inhibition on cytochrome P450 enzymes.

Poster Presentation : **MEDI.P-383**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Synthesis of Amlexanox Derivatives Using a Scaffold Hopping Approach

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Data Convergence Drug Discovery Research Center, Korea Research Institute of Chemical Technology, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*
[2]*Department of Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea*
[3]*Department of Chemistry, Yonsei University, Korea*

Amlexanox, which is used as a drug for recurrent aphthous stomatitis, asthma, and allergic rhinitis, has limitations in its moderate potency and poor solubility. In order to overcome the drawbacks, research on developing new alternative Amlexanox derivatives has been conducted. The objectives of these projects are on changing the peripheral functional groups except for changing the central structure. Unlike previously reported research, we sought to synthesize Amlexanox derivatives using the scaffold hopping strategy that changes the central structure of compounds. The new central structure commonly included in the synthesized compounds is pyridopyrimidine, a structure similar to quinazoline contained in the structures of a number of FDA-approved drugs. Although the synthesized compounds did not inhibit the original targets, TBK1 and IKKε, it was confirmed through kinase profiling analysis that they could selectively inhibit FLT4.

Poster Presentation : **MEDI.P-384**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Identification of *Mycobacterium tuberculosis* Rv3364c-derived small molecules for treatment of sepsis

Eunbi Lee, Kyungmin Kim, Sun-Joon Min[1,*]

Department of Applied Chemistry, Hanyang University, Korea

[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Sepsis is a global health problem that affects up to 50 million people each year as a result of a host response to a bacterial or microbial infection. Although great progress has been made in the understanding and treatment of sepsis, effective and targeted therapeutic strategies are still needed. The serine protease inhibitor Rv3364c, secreted from *Mycobacterium tuberculosis* (MTB), is highly expressed in cells during MTB exposure. Rv3364c inhibits the secretion of pro-inflammatory cytokines induced by LPS, a ligand of toll-like receptors 4 (TLR4), and binds to the Bin-Amphiphysin-Rvs (BAR) domain of sorting nexin 9 (SNX9), which is involved in intracellular trafficking. Thus, SNX9 is crucial in bacterial infection and inflammatory response, which suggests that inhibition of interaction between SNX9 and its associated protein is a viable molecular target for sepsis. On the basis of the structure of a key Rv3364c peptide motif ($_{12}$WLVSKF$_{17}$) binding to the BAR domain of SNX9, our drug discovery process, including virtual screening, hit identification, synthesis and optimization, led to the identification of 4-diamino-6-(4-*tert*-butylphenyl)-1,3,5-trazine ,**DATPT** as potential lead compound. Our compound showed improved potency in *in-vitro* functional assays compared to that of Rv3364c peptide fragment. Furthermore, it exhibited significant therapeutic effects in a mouse model of cecal ligation and puncture-induced sepsis. Therefore, peptide-derived small molecule could be a potential therapeutic candidate for the treatment of sepsis.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MEDI.P-385**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Design and synthesis of a SIRT 7 inhibitor with anti-cancer effect

Hak Hyun Lee, Jin Woo Choi[1], Kwang-Rok Kim[2], Hee Jung Jung[3,*]

College of Pharmacy, Drug Function, Chungbuk Natioanl University, Korea
[1]*College of Pharmacy, Biopharmaceutical Convergence Major, Sungkyunkwan University, Korea*
[2]*Korea Research Institute of Chemical Technology, Korea*
[3]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

SIRT7 deacetylates its substrates histone H3 (at lysine 18) and p53. p53, a tumor suppressor, lead to apoptosis or cell cycle arrest and is stabilized by acetylation. p53 deacetylation at K382 by SIRT7 suppressed cancer cell growth by decreasing p53 activity. To develop a novel SIRT 7 Inhibitor (4), which was prepared in three steps. Compound (2) was formed by ring formation of starting material 2,3-diaminobenzonitrile (1), which was reacted with carbonyldiimidazole reagent. Compound (3) was obtained by chlorination, which was reacted by nucleophilic attack with phosphorus oxychloride. Finally, compound (4) were obtained by SN2 type amination, which was reacted with various amino functional groups. Many compounds showed good IC50 values and relationship between the structure and antitumor activity will be discussed.

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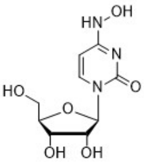
Poster Presentation : **MEDI.P-386**
Medicinal Chemistry
Event Hall THU 11:00~13:00

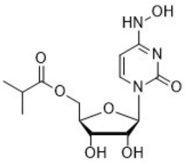
Synthesis and antivirial evaluation of β-D-N^4-hydroxycytidine (NHC) prodrug against RNA virus in vitro

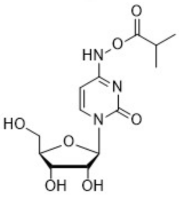
Yeon Jin An, Se Myeong Choi, Eun Rang Choi, Ye Eun Nam, Eun Woo Seo, Jong Hyun Cho*

Department of Health Science, College of Health Science, Dong-A University, Korea

As the pyrimidine nucleoside, β-D-N^4-hydroxycytidine (NHC, EIDD-1931) analogs have exhibited a broad spectrum of antiviral activity against RNA viruses including SARS-CoV, MERS-CoV, norovirus, chikungunya virus, Yellow FV, WNV, JEV, and Zika virus.[1] The novel NHC prodrug (CD-I-199) was synthesized as modification of MK-4482 (EIDD-2801)[2,3], which is currently using a treatment of global pandemic SARS-CoV-2 infection.[4] The NHC prodrug showed portent antiviral activities against SARS-CoV-2 (EC_{50} 3.5 μM), Flu A (H1N1: EC_{50} 5.8 μM and H3N2: EC_{50} 7.3 μM), Flu B (EC_{50} 3.4 μM) and Dengue (EC_{50} 3.95 μM) in vitro.


NHC(EIDD-1931)


MK-4482(EIDD-2801)


CD-I-199

Poster Presentation : **MEDI.P-387**

Medicinal Chemistry

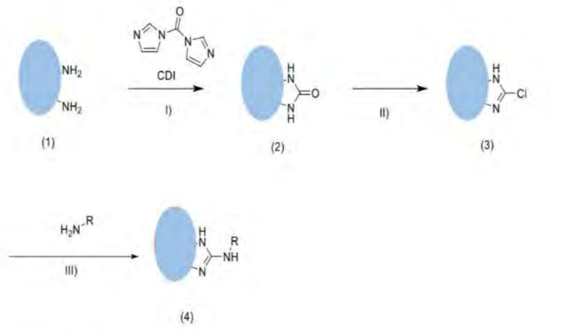
Event Hall THU 11:00~13:00

Synthesis and Anti-tumor Effect of a Novel class of SIRT7 Inhibitors

Jin Woo Choi, Hak Hyun Lee[1], Kwang-Rok Kim[2], Sang Jeon Chung[3], Hee Jung Jung[4,*]

College of Pharmacy, Biopharmaceutical Convergence Major, Sungkyunkwan University, Korea
[1]*College of Pharmacy, Drug Function, Chungbuk Natioanl University, Korea*
[2]*Korea Research Institute of Chemical Technology, Korea*
[3]*College of Pharmacy, SungKyunKwan University, Korea*
[4]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

SIRT7 deacetylates histone H3 and p53 which is a tumor suppressor. p53 is stabilized by acetylation and induces cell apoptosis or cell cycle arrest. So, we synthesis a novel SIRT7 enzyme inhibitors. To develop anti-tumor effect of a novel class of SIRT7 Inhibitors, we synthesized final product (4), which was synthesized in three steps from starting material (1). Product (2) was synthesized by cyclization using CDI (carbonyldiimidazole). Product (3) was obtained by chlorination of (2) that was reacted using $POCl_3$ (Phosphoryl chloride). Finally, we obtained the final product (4) through amination reaction using various amine reagents in 2-chloro position and showed good IC_{50} values.



I) CDI, DMF, rt 12h
II) $POCl_3$, 110 °C, 2 h
III) amine reagent, EtOH, 120 °C, overnight

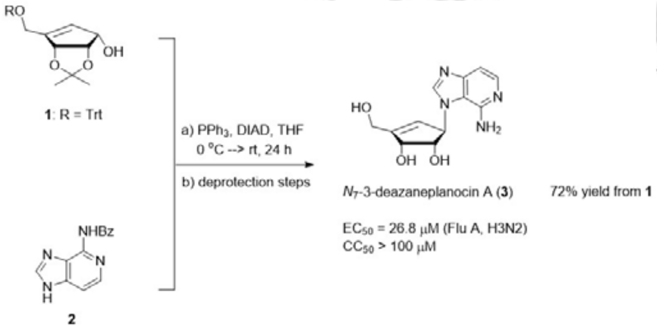
Poster Presentation : **MEDI.P-388**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Regioselective Synthesis of 3-Deazaneoalnocin A Derivatives and their Antiviral Activity against Influenza A Virus

Se Myeong Choi, Yeon Jin An, Eun Rang Choi, Ye Eun Nam, Eun Woo Seo, Jong Hyun Cho*

Department of Health Sciences, College of Health Sciences, Dong-A University, Korea

An efficiently regioselective synthesis of N_7-3-deazaneplanocin A have been developed by using Mitsunobu reaction.[1] Chiral cyclopentenol moiety (**1**) was synthesized with 33% overall yield from D-ribose using selective and practical method in total 8 steps.[2] N^6-Bz-3-deazapurine (**2**) was synthesized with 27% overall yield from 4-amino-2-chloropyridine in total 7 steps.[3,4,5] The coupling reaction of **1** with N^6-Bz-3-deazapurine (**2**) afforded N_7-3-deazaneplanocin A derivative in the presence of DIAD, PH_3P in THF without detection of the N_9-isomer in excellent yield. After removal of all protection groups, $N_7$3-deazaneplanocin A (**3**) was obtained in 72% yield from **1**. Invitro assay, N_7-3-deazaneplanocin A (**3**) exhibited mild activity against Flu A (H1N1) (EC_{50} 38.5 μM), Flu A (H3N2) (EC_{50} 26.8 μM) without cytotoxicity.



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Poster Presentation : **MEDI.P-389**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Pyrazolo[3,4-d]pyrimidin-1-yl piperidine derivatives as Bruton's tyrosine kinase inhibitors

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[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*
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Bruton's tyrosine kinase plays key role in B cell differentiation, proliferation, and survival. B cell receptor regulates the B cell's fate and cytokine release of B-lineage lymphoid leukemia cells. 4,6-Disubstitutes pyrazolo[3,4-d]pyrimidine derivatives were explored as irreversible Bruton's Tyrosine kinase (BTK) inhibitors. The structure-activity relationship was established with designed compounds to determine initial hit compounds, based on activities against BTK enzyme and TMD8 cells. In this report, we synthesized a series of pyrazolo[3,4-d]pyrimidine derivatives that were substituted with diphenyl moieties and evaluated BTK kinase inhibitory activity and cell based proliferation assay. Some of the compounds displayed excellent activity in vitro enzymatic and cell-based assay and structure-activity relationship of the substituents, and biological data and preliminary pharmacological data will be presented.

Poster Presentation : **MEDI.P-390**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Novel peptide synthesis technology applicable to Dna Encoded Library

Taeeun Kim, Sang Jeon Chung[1,*]

Biopharmaceutical Convergence, Sungkyunkwan University, Korea
[1]*College of Pharmacy, SungKyunKwan University, Korea*

Solid-phase peptide synthesis (SPPS) involves the continuous addition of protected amino acid derivatives to a growing peptide chain immobilized on the solid phase. And currently , Merrifield’s SPPS method is the most common method used in DNA Encoded Solid Phase Synthesis. DNA-Encoded Library (DEL) technology enables rapid, enconomical synthesis and exploration for novel chemical space. However, the current method has limitation in applying it to a DNA encoded library in a broader way. The challenge is that there is fatal limitations that the method currently used for synthesis affects DNA. In this reason, we develop a novel peptide synthesis method to overcome the limitation. As a result, it shows large potential by bringing the result of synthesizing peptides in a faster time without affecting DNA. This novel peptide synthesis method and application in Solid phase peptide synthesis can be applied to a larger range in the DNA encoded library and is expected to have more applications.

Poster Presentation : **MEDI.P-391**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Structure-activity relationship (SAR) studies of novel GSPT1 degrader

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Data Convergence Drug Research Center, University of Science & Technology, Korea
[1]*Department of chemistry, Sungkyunkwan University, Korea*
[2]*CHEMISTRY, The Catholic University of Korea, Korea*
[3]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Recent studies showed that Molecular glue degrader such as lenalidomide and pomalidomide bind to CRBN, a substrate receptor of CRL4 E3 ligase, to induce the ubiquitination and degradation of IKZF1 and IKZF3 in multiple myeloma cells, contributing to their anti-myeloma activity.In this study we explored novel GSPT1 small molecule degrader utilizing benzotriazinone scaffold that was previously discovered as a new CRBN binderParticularly, we examined structure-activity relationship analysis by exploring the position of ureido group on benzotriazinone scaffold, substitution on phenylureido group and benzylic substitution on benzotriazinoneAs the result, we identified 15f (TD-522) which exhibits strong anti-proliferative effect in both KG-1 (CC50 = 0.5 nM) and TMD-8 (CC50 = 5.2 nM) cell lines. Compound 15f effectively induced GSPT1 degradation with DC50 of 0.223 M and Dmax of > 95% at 10 nM concentration in KG-1 cells. In vivo xenograft study showed that compound 15f effectively suppressed TMD8-driven tumor growth, similar to the extent of CC-885, suggesting that it could be used for a novel GSPT1 degrader development.

Poster Presentation : **MEDI.P-392**

Medicinal Chemistry

Event Hall THU 11:00~13:00

In situ Polymerization via Bioorthogonal Condensation in Mitochondria Controls Cell Fate

Gaeun Park, Ja-Hyoung Ryu[1,*]

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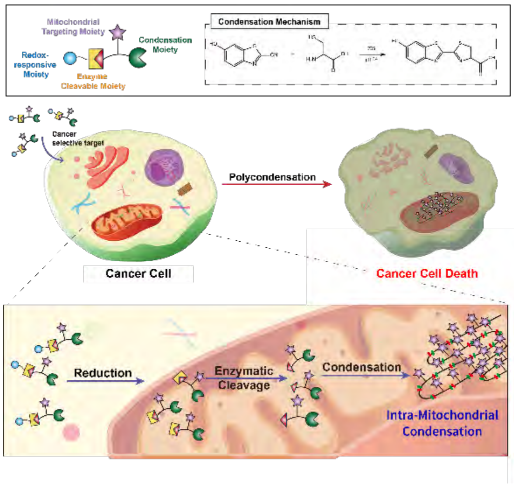
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Living organisms are composed of natural and functional nanomaterials including DNA, protein, and lipid membrane. Nanomaterials have a crucial role, interact with cell components and sometimes control cell fate. In biomedical applications, artificial nanomaterials have been designed to mimic biological materials in living systems. However, the main challenge of the nanomaterials is a low delivery efficiency due to poor tissue distribution and immune response under physiological barriers. Thus, in situ self-assembly or polymerization have been studied to construct nanomaterials in living systems. Bioorthogonal condensation is one of the strategies for in situ nanomaterial construction inside a complex biological environment. These reactions are fast, highly selective, and can be regulated by physiological stimuli such as pH, reductive environment, and enzyme activities.Herein, we presented a smart in situ polymerization system via bioorthogonal condensation between 2-cyanobenzothiazole(CBT) and Cysteine(Cys). We hypothesized that, while monomers in cytosol generally form dimers, the highly accumulated monomers within specific organelle can undergo polycondensation and form polymers in a concentration-dependent manner. In this work, we proved in situ polymerization induced by mitochondrial localization constructs nanomaterials in cells and this intra-mitochondrial polymerization controls cellular fate. Therefore, we expect in situ polymerization system would be widely applied in biomedical applications including cancer treatment.


Mitochondrial Targeting Moiety
Condensation Moiety
Redox-responsive Moiety
Enzyme Cleavable Moiety
Condensation Mechanism
Cancer selective target
Polycondensation
Cancer Cell
Cancer Cell Death
Reduction
Enzymatic Cleavage
Condensation
Intra-Mitochondrial Condensation

Poster Presentation : **MEDI.P-393**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Investigation of thioacetal-lipoic acid-ethyl piperidine compounds for cholinesterase inhibitors

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Division of Applied Chemistry & Biological Engineering, Hanbat National University, Korea

Based on the cholinergic theory for the treatment of Alzheimer's disease (AD), we reported the amide derivatives of lipoic acid and ethyl piperidine had an inhibitory effect on acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE). Alpha -lipoic acid (ALA) is an organo-sulfur compound derived from carprylic acid. ALA is made in animals normally and is essential for aerobic metabolism. Also, it’s an essential reporting factor for mitochondrial respiratory enzymes and improves mitochondrial function. ALA is well known as an antioxidant and has further beneficial effects on neurodegenerative diseases such as AD, Parkinson's disease, and Huntington's disease. ALA has disulfide bonds and can be reduced to dithiol. In this study, for structure-activity relationship (SAR) coupling reaction between the reduced dithiol and aldehydes resulted in thioacetal compounds, which were converted to thioacetal-lipoic acid-ethyl piperidine amide compounds. Compounds 15 (IC_{50} = 0.79 ± 0.29μM for AChE, IC_{50} = 0.66 ± 0.023μM for BuChE) showed better inhibitory activity than the positive control, galantamine (IC_{50} = 1.70 ± 0.9μM for AChE, IC_{50} = 9.4 ± 2.5 μM for BuChE).

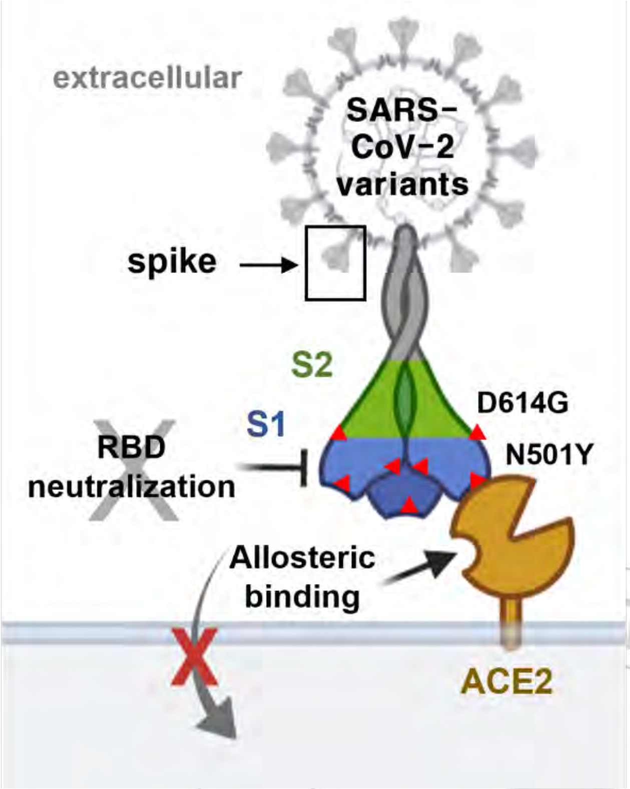
Poster Presentation : **MEDI.P-394**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Inhibition of ACE2-Spike Interaction by an ACE2 Binder Suppresses SARS-CoV-2 Entry

Young-Hee Shin, Kiyoung Jeong[1], Junhyeong Yim[2], Seung Bum Park[1,*]

Department of Chemical Engineering & Biotechnology, Korea Polytechnic University, Korea
[1]*Division of Chemistry, Seoul National University, Korea*
[2]*BioPhysics and Chemical Biology, Seoul National University, Korea*

The sudden emergence and rapid spread of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) have posed a serious global public health emergency. The rapidly generated variants of SARS-CoV-2 hamper the development of effective therapeutics and vaccines in the middle of the ongoing coronavirus disease 2019 (COVID-19) pandemic. Here, we have identified a novel small molecule that inhibited the interactions between SARS-CoV-2 spike RBDs and human receptor ACE2 by modulating ACE2 without impairing its enzymatic activity necessary for normal physiological functions. Furthermore, the identified compounds suppressed viral infection in cultured cells by inhibiting the entry of ancestral and variant SARS-CoV-2. They also showed the synergistic effect with Remdesivir(RDV), an FDA-approved drug with an orthogonal mechanism (viral replication/ transcription inhibition). Our study suggests that targeting ACE2 could be a novel therapeutic strategy to inhibit SARS-CoV-2 entry into host cells and prevent the development of COVID-19.



extracellular
SARS-CoV-2 variants
spike
S2
S1
D614G
N501Y
RBD neutralization
Allosteric binding
ACE2

Poster Presentation : **MEDI.P-395**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Targeting the Nuclear Receptor-Binding SET Domain Family of Histone Lysine Methyltransferases for Cancer Therapy: Recent Progress and Perspectives

Nayeon Kim, Su-Jeong Lee, Hongchan An*, Jungwook Chin*

New Drug Development Center, Daegu Gyeongbuk Medical Innovation Foundation, Korea

Nuclear receptor-binding SET domain (NSD) proteins are a class of histone lysine methyltransferases (HKMTases) that are amplified, mutated, translocated, or overexpressed in various types of cancers. Several campaigns to develop NSD inhibitors for cancer treatment have begun following recent advances in knowledge of NSD1, NSD2, and NSD3 structures and functions as well as the U.S. FDA approval of the first HKMTase inhibitor (tazemetostat, an EZH2 inhibitor) to treat follicular lymphoma and epithelioid sarcoma. This perspective highlights recent findings on the structures of catalytic su(var), enhancer-of-zeste, trithorax (SET) domains and other functional domains of NSD methyltransferases. In addition, recent progress and efforts to discover NSD-specific small molecule inhibitors against cancer-targeting catalytic SET domains, plant homeodomains, and proline-tryptophan-tryptophan-proline domains are summarized.

Poster Presentation : **MEDI.P-396**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Discovery of a Small-Molecule Degrader of Nonstructural Protein 1 of SARS-CoV-2

Wan Gi Byun, Seung Bum Park*

Department of Chemistry, Seoul National University, Korea

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is a highly pathogenic and transmissible strain of betacoronavirus that causes the coronavirus disease 2019 (COVID-19) pandemic which threatens global public health and economy. Despite an enormous research effort over the last 2 years, only a few therapeutics are available to date. Therefore, an unique therapeutic strategy for treating SARS-CoV-2 is still in urgent need. Nonstructural protein 1 (Nsp1), the first protein produced from the viral genome, plays a key role in inhibition of host immune responses and cellular replication of SARS-CoV-2. Nsp1 suppresses the translation of host mRNAs by directly blocking mRNA entry tunnel of a 40S small ribosomal subunit, resulting in the downregulation of host immune responses against viruses. On the other hand, Nsp1 can recognize stem-loop 1 (SL1) of SARS-CoV-2 5′ UTR and selectively facilitate the translation of the viral RNA. Thus, targeting Nsp1 is a promising therapeutic strategy. We identified a novel small-molecule Nsp1 degrader, compound 1, using a luciferase assay-based screening system. 1 destabilized Nsp1 by directly interacting with Nsp1, and reduced the cellular level of Nsp1. In addition, 1 can restore cell viability and antiviral response suppressed by Nsp1. We expect that selective clearance of SARS-CoV-2 Nsp1 by 1 could be an efficient antiviral strategy to overcome COVID-19.

Poster Presentation : **MEDI.P-397**

Medicinal Chemistry

Event Hall THU 11:00~13:00

A novel core skeleton design and synthesis of *N*-alkyl-1'-(substituted sulfonyl)spiro[chromene-2,4'-piperidin]-6-amine derivatives as 5-lipoxygenase inhibitors

Lee Hwasung, Young-Chang Kim, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

5-Lipoxygenase (5-LO) is the key enzyme in the biosynthesis of leukotrienes, which modulates the acute inflammatory processes. 5-LO inhibitors can potentially be employed for the treatment of various inflammatory disorders. In this study, we have designed and synthesized new *N*-alkyl-1'-(substituted sulfonyl)spiro[chromene-2,4'-piperidin]-6-amine based library as potential and novel 5-LO inhibitors. In vitro results showed that several synthesized compounds exhibited high 5-LO inhibitory activity, in parallel with the inhibition of leukotriene B4 (LTB4) production in the rat basophilic leukemia (RBL-1) cells. Among the synthesized compounds, *N*-(3-methoxybenzyl)-1'-tosylspiro[chromene-2,4'-piperidin]-6-amine (8l) was selected for in vivo study using a mouse ear edema model. Oral administration of 8l (100 mg/kg) inhibited arachidonic acid-induced ear edema, myeloperoxidase (MPO) activity, and LTB4 synthesis. SAR analysis and molecular docking studies demonstrated the allosteric binding mode between 5-LO and the synthesized compounds including 8l. In summary, the novel lead compound 8l was identified as a 5-LO inhibitor and will be employed for further investigation.

Poster Presentation : **MEDI.P-398**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Design and synthesis of 5-((2-methylbenzyl)thio)-1,3,4-thiadiazole-2-amine derivatives as a novel drug-like libraries

Ye Jin Shin, Dong Kyun Han, Lee Hwasung, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

A synthesis is designed around 5-((2-methylbenzyl)thio)-1,3,4-thiadiazole-2-amine based library. We focused on 1,3,4-thiadiazole because there is a possibility that can be used as drugs. For example, thiadiazole derivatives have been found to have the same effect through different mechanisms from Gleevec, which is famous as a treatment for Chronic Myeloid Leukemia. No matter how excellent a drug is, such as Gleevec, the effect is not perfect, such as recurrence or resistance of the disease. So discovering new drugs to increase options for specific disease treatment is very important. Paying attention to this importancy, we synthesized several derivatives of our core skeleton 1,3,4-thiadiazole by acylation and isocyanation. The synthesis starts from the alkylation at 2-thiol site of 5-amino-1,3,4-thiadiazole-2-thiol using 1-(chloromethyl)-2-methylbenzene as reagent. The resulting 5-((2-methylbenzyl)thio)-1,3,4-thiadiazol-2-amine was treated with KOH in EtOH. Both isocyanation and acylation occurred at amine site of 5-((2-methylbenzyl)thio)-1,3,4-thiadiazole-2-amine. First of all, the isocyanation reaction proceeded under 1.1eq of reagent using dichloromethane 5ml as solvent. Acylation reaction proceeded under 1.5eq of reagent using dichloromethane 5ml as solvent and added diisopropylethylamine (DIPEA). We performed High Performance Liquid Chromatography after extraction. To predict if they were likely to be used as oral drugs, we calculated Lipinski's "Rule-of-five". And most of the products were satisfied and we expect that among them there are candidates that can become drugs with outstanding efficacy.

Poster Presentation : **MEDI.P-399**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Design, synthesis, and biological evaluation of N-(2,7-Dimethyl-2-alkyl-2H-chromen-6-yl)sulfonamide derivatives as selective serotonin 5-HT6 receptor antagonists

Young-Chang Kim, Lee Hwasung[1], Young Dae Gong[*]

Department of Chemistry, Dongguk University, Korea
[1]*Dongguk University, Korea*

Serotonin 5-HT6 receptor, which is predominantly expressed in the central nervous system, is a valuable therapeutic target. Serotonin 5-HT6 receptor antagonists have potential for the treatment of various diseases that include psychotic disorders, dementia, depression, and obesity. In this study, we designed and synthesized the N-(2,7-dimethyl-2-alkyl-2H-chromen-6-yl)sulfonamide-based library as a potential serotonin 5-HT6 receptor antagonist. The library was subjected to a series of binding affinity tests to identify the lead compound, and check the selectivity of test compounds towards the 5-HT6 receptor. Accordingly, compound N-(2,2,7-trimethyl-2H-chromen-6-yl)naphthalene-2-sulfonamide was identified as the most active compound, with IC50 = 87 nM. The binding affinity of 95.3% of N-(2,2,7-trimethyl-2H-chromen-6-yl)naphthalene-2-sulfonamide (10 M) with the 5-HT6 receptor among other serotonin 5-HT1a, 5-HT2a, 5-HT2c, and 5-HT7, and dopamine receptors D1, D2, D3, and D4, demonstrated the high selectivity of N-(2,2,7-trimethyl-2H-chromen-6-yl)naphthalene-2-sulfonamide towards the 5-HT6 receptor.

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Poster Presentation : **MEDI.P-400**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Construction of a drug-like (3-methylbenzofuran-2-yl)(piperazin-1-yl)methanone Libraries toward Anti-Cancer Agent

Ji-Yeon Kim, Eun Hyo Lee, Sung Mi Baek, Young-Chang Kim, Young-Chang Kim, Young Dae Gong[*]

Department of Chemistry, Dongguk University, Korea

Benzofuran core, which is prevalently found in pharmaceutically active natural products, is an attractive structure in medicinal chemistry. Benzofuran derivatives have potential for the inhibition of various receptors including HIF-1α, Topoisomerase, HDAC, GSK-3β, mTOR, PEP, 5-HT1A, GPCR-40. These denotes pharmaceutical potentiality for nervous diseases therapy, anti-cancer, and diabetes restraining.Because of the structural similarity with purine, benzofuran also can be a DNA base-biomimetics. Therefore, we expect less toxicity, high bioavailability and affinity compared with cores that are not naturally found.In this study, we designed and constructed the (3-Methylbenzofuran-2-yl)(piperazin-1-yl)methanone-based library as a potential anti-cancer agent. The library was designed to satisfy Lipinski's rule of five; No more than 5 HBD, 10 HBA, 10 rotatable bonds; Less than 500 Daltons for MW; Does not exceed 5 for log P-value.

Poster Presentation : **MEDI.P-401**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Development of Small-Molecule STING Activators for Cancer Immunotherapy

Hyejin Kim*, Seongman Jo[1]

Infectious Diseases Therapeutic Research Center, Korea Research Institute of Chemical Technology, Korea

[1]*Department of Pharmacy, Infectious Diseases Therapeutic Research Center, Chungnam National University, Korea Research Institute of Chemical Technology, Korea*

Stimulator of interferon genes (STING) is a receptor on the surface of an endoplasmic reticulum and is activated by detecting pathogen-derived- or self-DNA in the cytoplasm. Activation of STING triggers innate immunity inducing secretion of typeI interfereons and other cytokines. Herein, we report a new compound, KAS-08 as the synergistic activator for STING. Through a high-throughput screening, we found an initial hit compound, and a following synthesis of the focused library revealed the optimized compound, KAS-08. KAS-08 showed cGAMP-dependent activity in STING-mediated immune response, which eventually provided anticancer activity in mouse tumor models. The synergistic effect of cGAMP-mediated immunity and efficient anti-cancer effects successfully suggests the therapeutic potential of KAS-08 for combination therapy in cancer treatment.

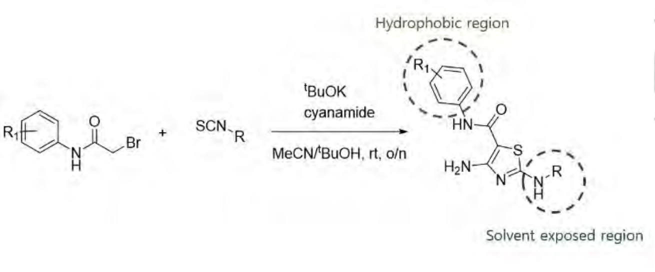
Poster Presentation : **MEDI.P-402**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Design and Synthesis of Aminothiazole based Anticancer Targeting CDK9

<u>Jong Woo Yoon</u>, Eunyoung Yoon[1], Seong Hwan Kim[1], Jung-Nyoung Heo[1,*]

Graduate School of New Drug Discovery and Development, Chungnam National University, Korea
[1]*Therapeutics and Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

CDKs (cyclin dependent kinase) are known as important cell cycle regulators and well-known highly promising and attractive strategy for the development of anticancer drugs. Among them, CDK9 has been observed in various hematological and solid malignancies, making it a valuable target for anticancer.Here, we designed and synthesized CDK9 selective inhibitor including aminothiazole scaffold. Aminothiazole has been known as one of the important CDK9 target compound. To increased the activities of the inhibitor, we used variety substituted aminothiazole group of solvent exposed region and replacing the variety substituted benzene group of hydrophobic region. Futher isozyme assay showed that our designed compounds were highly selective CDK9 inhibitor over other CDKs.



Poster Presentation : **MEDI.P-403**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Construction of chemical libraries based on the immunomodulatory drugs (IMiDs) for molecular glue degrader

Eunyeong Kim, Akshay Takwale[1], AhRa Go[1], Jong Yeon Hwang[1,*]

Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea

[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

The immunomodulatory drugs (IMiDs), lenalidomide, pomalidomide, CC-885, etc., bind to cereblon E3 ligase and repurpose the protein for new PPI interaction leading to the ubiquitination of substrate (IKZF1, IKZF3, CK1α, and GSPT1) and subject to the proteasome for degradation. In this study, we tried to construct a series of novel neo-substrate protein degraders by conjugating the amino acids with the well-known CRBN binder. These compounds were evaluated through cytotoxicity assay in AML (KG-1) cell line. In addition, we did a degradation study using HiBit assay. The results acquired from the degradation assay with a few analogs reflect the moderate degradation of known neo-substrates. In this poster, we'll discuss detailed experimental results about our approach.

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Poster Presentation : **MEDI.P-404**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Copper-Mediated Three-Component Reaction for the Synthesis of *N*-Acylsulfonamide on DNA

TaeYeon Kwon, Minwoo Choi[1], Jaehoon Sim[1,*], Hyunjin Kim[2,*]

Department of Pharmacy, Chungnam National University, Korea
[1]*College of Pharmacy, Chungnam National University, Korea*
[2]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

DNA-encoded library (DEL) was first proposed by Brenner and Lerner in 1992. DEL is a collection of small molecules covalently linked to DNA code that reflects structural information about a compounds. Although it has emerged as a new paradigm that surpasses combinatorial chemistry, due to the property of DNA, the use of existing organic synthesis methods is limited. For example, acidic conditions can depurinate DNA, and high temperatures and radical reactions can cause damage of DNA barcodes. Due to the limitations of the reactions applicable to these DEL, it is necessary to develop a new synthetic methodology. In this study, we developed a three-component-reaction of *N*-acylsulfonamide containing various functional groups as a novel synthesis method for DEL.

Poster Presentation : **MEDI.P-405**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Sphingosine Backbone Modified β-Glucosylceramide Analogues Demonstrate a Role of Lipid Structure in Mincle Activation

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Department of Chemistry, Seoul National University, Korea
[1]*BioPhysics and Chemical Biology, Seoul National University, Korea*
[2]*Division of Chemistry, Seoul National University, Korea*

Macrophage inducible C-type lectin (Mincle) is a C-type lectin receptor which recognizes both pathogen- and damage-associated molecular patterns. Because of its proinflammatory response against various molecules, Mincle has attracted attention as a promising target of vaccine adjuvant and anticancer drugs. Recently, β-glucosylceramide has been discovered as a novel endogenous Mincle ligand which is constituted of two lipid chains, an acyl chain and a sphingosine chain. An effect of the acyl chain in Mincle activation has been reported by comparing natural β-glucosylceramide analogues. However, a sphingosine backbone modified derivatives has not been explored yet. Here, sphingosine modified β-glucosylceramide analogues were chemically synthesized to examine the relationship between the lipid structure and Mincle activation. Ligand-receptor interactions were evaluated by computational docking assay and reporter gene assay. As a preliminary result, an isomerization of double bond of sphingosine showed higher docking scores and Mincle activation. Also, terminal branching of sphingosine affected the ligand-receptor interactions. In summary, we expect to discover a more potent Mincle ligand than previously reported agonists.

Poster Presentation : **MEDI.P-406**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Total synthesis of Duocarmycin analogue involving dual alkylating unit as a potent ADC payload

Eunseok Choi, Hyuna Park, Sang Jeon Chung[1,*]

Biopharmaceutical Convergence, Sungkyunkwan University, Korea
[1]*College of Pharmacy, SungKyunKwan University, Korea*

Antibody-drug conjugates (ADCs) are promising anticancer agents that can selectively deliver a cytotoxic payload to targeted cancer cells. In order to improve an ADC's therapeutic index, the necessity of investigating a more potent payload has been addressed. Duocarmycins, composed of a DNA alkylating unit and a binding unit responsible for directly binding with and alkylating adenine, exhibited a remarkable anticancer effect, but also displayed hepatotoxicity and bone marrow suspension. Therefore, we introduced the ADC platform into Duocarmycins to reduce their side effects while maintaining their outstanding anticancer effects. We also established a retrosynthetic strategy to synthesize a prodrug of a Duocarmycin analogue featuring a dual alkylating unit. This Duocarmycin analogue was partitioned into three moieties. Each moiety includes an indole ring substructure constructed with a Heck reaction, and the key enantioselective structure of the DNA alkylating units are synthesized with a ring-opening reaction of a chiral epoxide.

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Poster Presentation : **MEDI.P-407**
Medicinal Chemistry
Event Hall THU 11:00~13:00

A one-pot synthesis of pyrroloisoquinolines and evaluation of their anti-cancer activities

Santosh shivanand Raikar, Hoyeong Park, Pilho Kim[1,*]

Medicinal Chemistry, University of Science & Technology / KRICT, Korea
[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Pyrroloisoquinoline (PIQ) scaffold is known to have remarkable biological activities including antiviral and antitumor activities. Several PIQ alkaloids, such as crispene-A and lamellarin D, have been proved to be cytotoxic to cancer cells. Crispine-A alkaloid, isolated from Carduus crispus, has significant anti-tumor activities against KB, SKOV3, and HeLA cell lines. In addition, some of the PIQ analogs have been characterized as inhibitors of phosphodiesterase 10A, exhibiting encouraging efficacies to overcome diseases related to antineoplastic, hypotensive, sympatholytic, and psychotropic, and psoriasis. Herein, we will discuss a one-pot protocol for the synthesis of PIQ-containing derivatives. Anti-cancer activities of the PIQs prepared will be also presented against diverse cancer cell lines.

Poster Presentation : **MEDI.P-408**
Medicinal Chemistry
Event Hall THU 11:00~13:00

FBLD: Development of selective HDAC6 inhibitors

Eunhye Lee, Yujin Park, Sejin Jung, Dongwan Kang, Minwoo Kim, Seungik Jeong, Hyeongcheol Ham, Soong-Hyun Kim*

Department of Medicinal Chemistry, Korea Medical Develop Innovation hub (K-MEDI hub), Korea

In 2011, Pellecchia group demonstrated that the techniques of fragment-based lead discovery (FBLD) could be applied to find proper metal binding pharmacophores targeting metallo-proteins. Histone deacetylases (HDACs) are one of the representative metallo-proteins as an epigenetic target enzyme. Histone deacetylase 6 (HDAC6), especially, has a structurally distinct feature among HDAC isoforms and has been considered as an important target for the treatment of diverse diseases including cancer, neurodegenerative diseases, autoimmune disorders, drug addiction, viral infection, and rare diseases. In order to develop novel HDAC6-selective inhibitors, we employed a fragment-growing strategy. Firstly, we performed a virtual screening using an open database of ZINC 15 to select a major capping fragment, calculated in the surface and channel region of HDAC6 enzyme. On the selected fragment, we installed a well-known zinc binding group (hydroxamic acid), which chelates a zinc ion in the catalytic domain of the enzyme. This approach generates our hit compound, possessing a potent activity (IC50 = 56nM for HDAC6) and great selectivity (e.g. 16 > HDAC6/HDAC1) over other HDAC isoforms. Next, maintaining the key interactions of the hit compound with HDAC6 enzyme, we rationally designed and screened the modified capping units to obtain an initial lead compound with both improved potency (IC50 = 6.6nM for HDAC6) and selectivity (e.g. 56 > HDAC6/HDAC1). Having the optimized capping fragment intact, we then optimized the zinc binding group subsequently. Analysis of the reported zinc binding modes in literatures and modifications to enhance the binding affinity gave rise to an advanced lead compound with the similar potency (IC50 = 6.7nM for HDAC6) and even greater selectivity (e.g. 319 > HDAC6/HDAC1). Currently, lead optimization and further studies for therapeutic evaluation are on-going in our institute. Entire FBLD stories and other research results will be described in this poster.

Poster Presentation : **MEDI.P-409**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Orally available Bruton’s Tyrosine Kinase (BTK) degrader with excellent in vivo efficacies against B-cell malignancies.

Vineetkumar bapusaheb Patil, Hoyeong Park[1], Ye Seul Lim[2], Han Wool Kim[3], Je Ho Ryu[4], Song Hee Lee[5], Pilho Kim[6,*]

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Bruton’s Tyrosine Kinase (BTK) is one of the validated drug targets for the treatment of B-cell mediated cancers, such as chronic lymphocytic leukemia (CLL) and mantle cell lymphoma (MCL). BTK triggers the B-cell receptor (BCR) signaling cascade, which eventually contributes to the growth and survival of leukemic cells, hence, inhibiting this pathway could be an ideal way to reduce the tumor accumulation. Three BTK inhibitors, Ibrutinib, Acalabrutinib and Zanubrutinib, have been approved by the US FDA for the treatment of MCL and CLL. However, due to the C481 mutations in the ATP binding pocket of BTK, the patients treated with Ibrutinib acquire resistance that leads to tumor progression. Therefore, a novel approach is required to overcome this resistance issue, such as reversible inhibitors and PROteolysis-TArgeting Chimera (PROTAC). PROTAC has been successfully utilized to degrade BTK, thereby inactivating the BCR signaling and leading to tumor suppression in animal models. Currently, clinical trials are underway with a few BTK degraders, such as NX-2127 and BGB-16673. Through our continuous exploration on BTK degraders, PROTAC-82 was recently found out as an orally available BTK degrader, which showed excellent pharmacokinetics and in vivo efficacy against both wild type and mutant BTKs, compared with ibrutinib and a known BTK degrader, MT-802. The biological data of PROTAC-82 will be presented.

Poster Presentation : **MEDI.P-410**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis of Novel Tetrahydroisoquinoline-pyrimidines as Potential Inhibitors of Mycobacterial Cell Wall Biosynthesis

Mingi Chu, Heeseung Lim[1], Ji Hye Choi[1], Eomjeong Kang[1], Clifton E. Barry 3rd[2], Ill young Lee[1,*]

Targeted Cancer Drug Team, Department of Medicine and Chemistry, Daegu Gyeongbuk Advanced Medical Industry Promotion Foundation (k-medihub), Korea

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[2]*Tuberculosis Research Section, National Institute of Allergy and Infectious Diseases, United States*

Tuberculosis (TB) is a major global health problem, and there is an urgent need to discover new agents with improved efficacy and safety and shorter treatment duration. Some drugs to treat tuberculosis can cause serious side effects, and the evolution of resistance patterns, including MDR and XDR, is making many drugs ineffective. Therefore, there is an urgent need to develop a therapeutic agent for tuberculosis, especially with a novel mechanism of action. We will discuss the Structure–activity relationship (SAR) results of a series of potent Tetrahydroisoquinoline-pyrimidines derivatives that have demonstrated activity against Mycobacterium tuberculosis (Mtb) H37R replication.

Poster Presentation : **MEDI.P-411**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Design and synthesis of 2-imidazoline derivatives for treatment of the Alzheimer's disease

Haheon Kim, Kooyeon Lee[1,*]

Department of Bio-Health Convergence, Kangwon National University, Korea
[1]*Department of Bio-Health Technology, Kangwon National University, Korea*

Alzheimer’s disease (AD) is a progressive neurodegenerative disorder that is characterized by dementia, cognitive impairment, and memory loss. Despite many efforts to develop medication for AD, effective treatment has not been developed yet. The 2-imidazoline derivatives have been known to have various beneficial activities anti-inflammatory, anti-hyperglycemic and anti-hypercholesterolemic, however, their potential as a medication for AD has not been investigated. In this study, we synthesized 2-imidazoline derivatives and evaluated their effects on cholinesterases (ChEs) activity and ROS-mediated neuronal damage. Most of compounds showed a concentration-dependent inhibition of acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) activities. 21 compounds (**3-23**) showed good efficacy in AChE inhibitory ability and 8 compounds (**3-23**) showed good efficacy in BuChE inhibitory ability. Among them, 8 compounds (**8, 14, 16-21**) had AChE and BuChE simultaneous inhibitory ability. In particular, compound **14** has the lowest AChE and BuChE inhibitory ability with IC_{50} values of 3.8 μM and 1.9 μM. Then, to evaluate the neuroprotective effect of the derivatives, we determined intracellular ROS level, in the presence of hydrogen peroxide. The generation of intracellular ROS by hydrogen peroxide was reversed by 12 compounds in SH-SY5Y cells, indicating that those compounds have neuroprotective effects. Thus, the 2-imidazoline derivatives have a great potential for treating AD due to their ability to inhibit ChEs and neuronal damage.

Poster Presentation : **MEDI.P-412**

Medicinal Chemistry

Event Hall THU 11:00~13:00

SAR study of small molecule inhibitors of STING-ligase interactions for cancer immunotherapy

Caroline Kim, Seung Bum Park[1,*]

Chemistry, Seoul National University, Korea

[1]*Division of Chemistry, Seoul National University, Korea*

Inhibitors of the protein-protein interaction (PPI) between stimulator of interferon genes (STING) and its E3 ligase, which negatively regulates the innate immune response against DNA viruses and cytosolic DNA, pose as potential immunotherapeutic agents. Normally, cGAMP is a dinucleotide that binds to cytosolic STING and stimulates robust immune responses. However, the low efficacy of cGAMP analogs in clinical trials presents a need for alternative therapies. A previous study revealed the hit compound 1 to be a potent inhibitor of the STING-E3 ligase PPI. A limitation of compound 1 is its poor solubility, thus structural modifications need to be made without diminishing its potency. In this work, 31 analogs of compound 1 were synthesized by varying mainly four substituents on the core skeleton structure (R0, R1, R2, and R3), and their activities were examined by measuring their PPI inhibitory activity, ability to enhance cytokine mRNA expression when co-treated with cGAMP, and effect on STING protein levels. The study identified several compounds with similar IC50 values as compound 1, some of which rendered cytotoxic effects. Among the analogs that did not compromise cell viability, we observed several that increased IFN-1 and IL-6 mRNA expression and increased STING protein levels. Our SAR study revealed that the R3 substituent is very important, the structure of which can lower inhibitory activity or upregulate cytokine transcription. These observations suggest a PPI modulation approach to upregulate proteins with immunotherapeutic potential. Overall, this study has implications for expanding the utility of known anticancer drugs by using a secondary targeted approach to potentiate the immunogenic effects of an endogenous therapeutic.

Poster Presentation : **MEDI.P-413**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Discovery of covalent TAK1 inhibitor: a molecular approach to cancer therapeutics

Jin Young Min, Eunjin Kook, Myeong A Choi[1], Ye-Mi Kwon[1], Jung Yeol Lee[1], Do-Hee Kim[*]

Department of Chemistry, Kyonggi University, Korea

[1]*Department of Pharmacy, Daegu Gyeongbuk Medical Innovation Foundation, Korea*

Transforming growth factor-β activated kinase-1 (TAK1) is serine/threonine kinase that can promote tumor cell survival/progression by modulation of apoptotic signaling and stress responses. TAK1 is a potential therapeutic target for cancers and inflammatory disease. We discovered novel acrylic acid derivatives, which were found to exhibit potent inhibitory effect against TAK1. This compound showed excellent in vitro kinase activity for TAK1 and anti-proliferative activity in various colon cancer cells. This compound may preferentially bind to the cysteine residue present in active site of TAK1. In addition, we found that knockdown of TAK1 attenuated cell proliferation via inhibiting Nrf2 signaling pathway in colon cancer cell lines. When compared with 5Z-7-oxo induced stronger apoptotic effects associated with increased suppression of Nrf2 signaling.Taken together, these findings suggest TAK1 inactivation through cysteine modification as a potential therapeutic approach for treatment of colon cancer.

Poster Presentation : **MEDI.P-414**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Synthesis and evaluation of Aurone derivatives as melanogenesis inhibitor

Jaekwon Kim, Kooyeon Lee*

Department of Bio-Health Convergence, Kangwon National University, Korea

Aurone, one of the flavonoids contained in natural plants, has various biological activities, including, anti-cancer, anti-oxidant, anti-inflammatory, anti-diabetic and neuroprotective activities. Hyperpigmentation is induced by the overactivation of tyrosinase, which is a rate-limiting enzyme in melanogenesis. Aurone derivatives are known to have inhibitory effects on tyrosinase, however, the relationship between the structure of aurone and its anti-melanogenesis activity is not yet identifeid. In this study, we synthesized 9 aurone derivatives substituted at C2`, C3`, C4` and C5`of the aurone backbone with hydrogen and hydroxyl functionalities by chemical synthesis. Compound **2**, **6**, **8** have tyrosinase inhibitory activity. Among them compound **6** showed highest anti-tyrosinase activity with IC_{50}value of 2.0 μM. The structure-activity relationship (SAR) study revealed that the coexistence of hydroxyl and methoxy at the C2` and C4` position is essential for tyrosinase and melanogenesis inhibitory activity. Thus, this study would be helpful for the development of tyrosinase inhibitor to regulate melanin synthesis and compound **6** might be useful in cosmetics as a skin-whitening agent.

Poster Presentation : **MEDI.P-415**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Discovery and SAR study of novel 2-Anilinoquinoline based arylamides as RAF inhibitors endowed with potent antiproliferative activity

Hyun Ji Kim, Ashraf.K El-Damasy[1,*], Gyo chang Keum[2,*]

Department of Chemistry, Sogang University, Korea

[1]*Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Egypt*

[2]*Creative Research Center for Brain Science, Korea Institute of Science and Technology, Korea*

Dysregulated phosphorylation by kinase results in serious diseases such as cancer. Therefore, discovering new chemical entities as inhibitors of the oncogenic kinases is a legitimate strategy for cancer treatment. In this regard, our group discovered two promising lead compounds, 9a and 9c, based on the 2-anilinoquinoline scaffold tethered with arylamide. Both 9a and 9c showed superior anticancer potencies compared with the FDA-approved drug Imatinib, with low micromolar/sub-micromolar GI50 values against diverse cancer cells including colon HCT-15, renal TK-10 and UO-3. Biochemical kinase assay of 9c revealed its selective and potent activity towards RAF kinase, with IC50 values of 0.888 uM and 0.229 uM over B-RAFV600E and C-RAF kinase, respectively. Prompted by these promising results, a SAR study using 9a and 9c as lead compounds is in progress, and the biological data of newly synthesized compounds showed much improved IC50 values against B-RAFV600E and C-RAF. This results will be hopeful for the development of novel B-RAFV600E and C-RAF inhibitors.

Poster Presentation : **MEDI.P-416**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery of Highly Potent Protein Degraders targeting Bruton’s Tyrosine Kinase

Yunha Choi, Ye Seul Lim[1], Vineetkumar Bapusaheb Patil[2], Je Ho Ryu[1], Song Hee Lee[3], Pilho Kim[4,*]

Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea
[1]*Research Center, Ubix Therapeutics, Korea*
[2]*Medicinal Chemistry, University of Science & Technology / KRICT, Korea*
[3]*UBIX THERAPEUTICS, Korea*
[4]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Bruton’s tyrosine kinase (BTK) is a member of the Tec kinase family that plays an important role such as the proliferation and survival in the B-cell receptor (BCR) signaling pathway. B-cell-related diseases can be caused by overexpression of BTK in B cells because they excessively stimulate BCR signaling pathway. Thus, the inhibition of BTK has been proven to be a practical way of treating diseases, such as chronic lymphocytic leukemia (CLL) and mantle cell lymphoma (MCL). Ibrutinib is an irreversible covalent BTK inhibitor with remarkable efficacies and survival rates in CLL and MCL patients. BTK inactivation occurs through covalent bonding of Michael acceptor part of ibrutinib to cysteine-481 (C481) residue of ATP binding domain in BTK. However, ibrutinib resistance has been reported mainly due to BTK C481 mutations. Because of the mutation of cysteine to serine (C481S), ibrutinib can no longer bind to BTK. To overcome the limitations of small molecule inhibitors, PROteolysis TArgeting Chimeras (PROTACs) have been emerged as novel approaches to induce degradation of the target protein. It has been reported that BTK-PROTACs could successfully target both wild-type and mutated BTKs, leading to clinical studies with several candidates, such as NX-2127 and HSK29116.The focus of our research has been discovery of novel BTK protein degraders with good efficacies and druggability. In a previous study by our group, a potent BTK degrader was discovered and evaluated both in vitro and in vivo. Based on the analysis of structure-activity relationship, the inhibitor part of BTK-PROTACs was explored to improve pharmacokinetics (PK) and pharmacodynamics (PD) profiles. The activity and druggability of the PROTACs prepared will be discussed such as degradation potency, metabolic stability, PK, and PD profiles.

Poster Presentation : **MEDI.P-417**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Synthesis of Acyclic Nucleoside Derivatives Based on Acyclovir and Ganciclovir

Eun Woo Seo, Eun Rang Choi, Se Myeong Choi, Yeon Jin An, Jong Hyun Cho[1,*]

Health science, Dong-A University, Korea
[1]*Medicinal Biotechnology, Dong-A University, Korea*

Novel acyclic five-membered base nucleosides as the combinational structure of ribavirin and acyclovir or ganciclovir were designed to find new hit and lead compounds against RNA virus in **Fig 1**. Acyclic nucleosides (**1**-**35**) were synthesized using two synthetic routes, either coupling reaction or click reaction. Mitsunobu reaction of acyclic sugar moieties (**1a**-**d**) with commercially available pyrazole, imidazole, triazole, followed by removal of protecting group(s) provided their corresponding nucleoside ester derivatives (**1**-**16**) in moderate to good yield. The nucleoside esters were treated with ammonia to afford the corresponding nucleoside analogs (**17**-**31**) in good yield. Additionally, 1,2,3-triazole-4-carboxylate analogs were prepared by click reaction (**32**,**33**). 1,2,3-triazole-4-carboxyl ester was treated with ammonia to give the 1,2,3-triazole nucleoside analogs (**34**,**35**) in good yield. Among them, the nucleosides (**17**) showed activity (EC_{50} 25 μM) against Flu A (H1N1) in **Fig 2**. The prepared nucleosides are under investigation of antiviral activity against the other RNA viruses.

Figure 1.

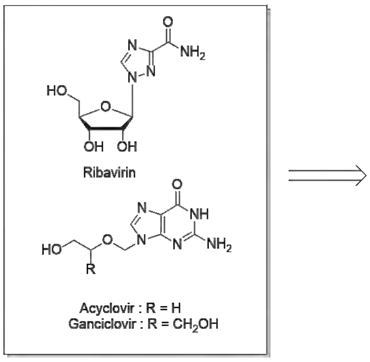
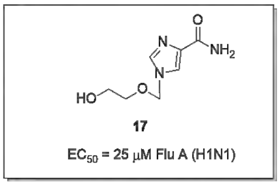


Figure 2.



Poster Presentation : **MEDI.P-418**

Medicinal Chemistry

Event Hall THU 11:00~13:00

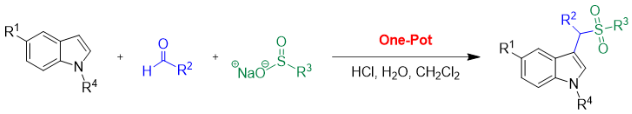
One-Pot Synthesis of Arenesulfonyl Indole Derivatives and Their Application in Alzheimer’s Disease (Cholinesterase Inhibitor) *in vitro* and *in vivo* Studies

Seungyeon Lee, Chanbin Lee, Kooyeon Lee[1,*]

Bio-Health Technology, Kangwon National University, Korea

[1]*Department of Bio-Health Technology, Kangwon National University, Korea*

Typical symptoms of Alzheimer's Disease (AD) include short-term memory loss and cognitive disorder. Indole derivatives have therapeutic effect such as antipsychotics. Herein, we describe a convenient One-Pot synthesis method and evaluation of cognitive function for arenesulfonyl indole derivatives. First, we developed simple One-Pot synthesis by adding HCl, H_2O, and solvent CH_2Cl_2 at start material to desired higher yield than previous methods and synthesized 34 compounds in a stable state. These compounds were evaluated by Ellman's colorimetric method for cholinesterase (ChE) inhibition and had high potential of cognitive function in eight compounds (*in vitro*). One of them was injected into scopolamine-induced mice to be efficient in passive avoidance test, and time to find a platform is reduced in water maze test to improve memory (*in vivo*). In Structure Activity Relationship (SAR), the improvement of the inhibition of ChE increased when the electron donating group was ortho-position and the electron withdrawing group was meta-position. In conclusion, we will synthesize additional derivatives by referring to molecular modeling and SAR. Most arenesulfonyl indole derivatives have been demonstrated by experiments that have improved cognitive function and there will be a potentially pharmacological development in preventing AD.



Poster Presentation : **MEDI.P-419**
Medicinal Chemistry
Event Hall THU 11:00~13:00

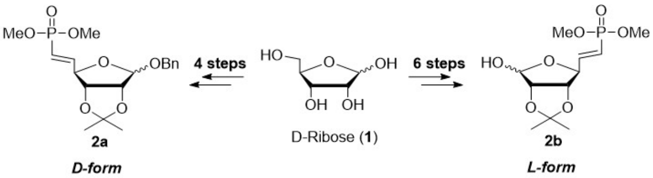
Efficient Synthesis of D-/L-Phosphonate Ribose Analogs using Cross Metathesis

<u>Ye Eun Nam</u>, Eun Woo Seo, Eun Rang Choi, Se Myeong Choi, Yeon Jin An, Jong Hyun Cho[1,*]

Health science , Dong-A University, Korea
[1]*Medicinal Biotechnology, Dong-A University, Korea*

The phosphonate D-/L-ribose analogs were efficiently synthesized by using the cross metathesis (CM) reaction. The key intermediates, D-/L-ribolactols, was prepared from D-ribose in 3 steps and 5 steps respectively. In the case of D-ribolactol, the oxidation of 5-OH with IBX and then wittig reaction after reaction of D-ribose with acetone followed by protection of 1-OH with benzyl group afforded protected D-4-vinylribolactol in quantitative yield. In the case of L-ribolacrol, the treatment of vinyl magnesium bromide after reaction of D-ribose with acetone and protection of its 5-OH with TBS provided a vinyl diol derivative. The next, subsequently the removal of the TBS with NH_4F and the oxidation of a 1,2-diol group with $NaIO_4$ gave L-4-vinylribolactol derivative in quantitative yield. The CM reaction of D-/L-4-vinylribolactol with dimethyl vinylphosphonate derivatives with a H-G catalyst II afforded their corresponding phosphonate derivatives in 60% yield (D-form, **2a**) and 70% yield (L-form, **2b**), respectively.

Figure1.



Poster Presentation : **MEDI.P-420**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Potent and stable microbial metabolite derivatives targeting aryl hydrocarbon receptor for the treatment of intestinal inflammatory diseases

Hansol Joo, Taeho Lee, Young Taek Han[1], Jong-Wha Jung*

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[1]*College of Pharmacy, Dankook University, Korea*

The aryl hydrocarbon receptor (AhR) is a ligand-activated transcription factor that belongs to the basic helix-loop-helix family of proteins. Whereas the AhR was initially deemed as a key regulator of xenobiotic-metabolizing genes, more recently, therapeutic and chemopreventive targeting of the AhR attracted attentions. A microbial metabolite of Thermosporothrix hazakensis, 2-(1' H-indole-3'-carbonyl)-thiazole-4-carboxylic acid methyl ester (ITE), is a putative AhR endogenous ligand. ITE was discovered as highly potent and non-toxic AhR agonist, and has been used in numerous in vitro and in vivo studies as a benchmark chemical regulation of AhR. Indothiazinone (indolyl thiazolyl ketone; ITZ), a structural analog ITE, was isolated from the cultures of novel Myxobacterial strain 706, belonging to the Sorangiineae new family. In addition, it was reported that the co-presence of ITE and ITZ in Thermosporothrix hazakensis SK20-1T cultures. Interestingly, ITE is a very potent AhR agonist exhibiting a single digit nanomolar activity, but it activates the AhR only transiently. It is probably due to the chemical lability of methylester moiety in the aqueous milieu containing non-specific esterases, and which is attributed to limiting the application of ITE in vivo. Thus, chemically as well as metabolically stable ITE analogs are required. Herewith, we report synthesis of a series of ITE and ITZ derivatives and evaluation of their effects on AhR activity for the treatment of intestinal inflammatory diseases.

Poster Presentation : **MEDI.P-421**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Antioxidative and Enzyme Inhibitory Activities of mixed Ishige okamurae extract and Wolfiporia extensa extract

Seonyeong Ahn*, **Mingyeong Kim[1],***, **Byong Wook Choi[2]**, **Bong Ho Lee[1]**

Department of Chemical and Biological engineering, Hanbat National University, Korea
[1]*Department of Chemical and Biological Engineering, Hanbat National University, Korea*
[2]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Generally, brown algae contain many secondary metabolites including polyphenols. Thus, they have diverse biological activities. Wolfiporia extensa (Peck) Ginns (syn. Poria cocos F.A.Wolf) is a fungus in the family Polyporaceae. It is a wood-decay fungus but has a subterranean growth habit. It also showed diverse bioactivities. Thus, we prepared the extracts of two natural resources and extracts mixture and evaluated their antioxidative and some enzyme inhibitory activities. The 70% ethanol extracts of Ishige okamurae and Wolfiporia extensa showed 77.5% and 73.1% radical scavenging activity at 1 mg/mL, respectively. The mixture of two extracts showed very similar radical scavenging activity showing no activity enhancing effect. The 70% ethanol extract of Wolfiporia extensa showed 85.1% elastase inhibitory activity at 1 mg/mL, but it showed very weak tyrosinase inhibitory activities unlike Ishige okamurae, which shows a strong tyrosinase inhibitory effect at the same concentration. The metabolites of the extracts were analyzed by high pressure liquid chromatography-mass spectrometry (HPLC-MS). Our study suggests that the above single or mixed extracts can be used as functional materials or cosmetics.

Poster Presentation : **MEDI.P-422**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Design, synthesis and evaluation of steroid mimics for the treatment of excessive steroid production

Jooyoung Seok, Changmin Oh, Ujjwala Karmacharya, Jong-Wha Jung*

College of Pharmacy, Kyungpook National University, Korea

Structural mimicry of endogenous ligands is one of the most important strategies in nature as well as drug discovery. Steroids have been utilized as fruitful skeletal sources for such a structural mimicry. Natural products from plants mimic the steroidal scaffold of estradiol, a vertebrate estrogen: an isoflavon genistein, a coumestan coumestrol, and a stilbene resveratrol are non-steroidal estrogen analogs. Synthetic estrogen analogs such as diethylstilbestrol and tamoxifen also mimic the steroidal structure. A common strategy for those mimicry is that the aromatic structures in their non-steroidal scaffolds mimic A or D rings of estradiol. Importantly, functional diversity and promiscuity of steroids imply potential expansions of similar approaches to the other steroids, such as cortisol. Herewith, we demonstrate steroid mimics inhibiting cortisol secretion. The small molecules inhibited early step of the steroid biosynthesis and cholesterol biosynthesis, and therefore, has potential of being used to develop new drugs to control excessive steroid production.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MEDI.P-423**

Medicinal Chemistry

Event Hall THU 11:00~13:00

[Withdrawal] Synthesis of Acyclic Nucleoside Derivatives Based on Acyclovirand Ganciclovir

Eun Woo Seo, Eun Rang Choi, Se Myeong Choi, Yeon Jin An, Ye Eun Nam, Jong Hyun Cho[1,*]

Health science, Dong-A University, Korea
[1]*Medicinal Biotechnology, Dong-A University, Korea*

- Withdrawal -

Poster Presentation : **MEDI.P-424**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Rational Design and Synthesis of Tunable Fluorophore Scaffold

Sihyeong Yi, Dahham Kim, Seung Bum Park*

Division of Chemistry, Seoul National University, Korea

Novel fluorescent core skeletons are in high demand for various biomedical studies and bioimaging applications. Despite being small (400 nm) and exhibit tunable emission wavelengths that cover the blue-to-red color range. Furthermore, dramatic changes in brightness in response to changes in polarity result in unique turn-on behavior in cellular lipid droplets. Due to their smallness and structural similarity, we used our fluorophore to prepare a fluorescent unnatural amino acid that exhibits the longest absorption and emission wavelengths reported to date, highlighting its applicability as a novel biological probe.

Poster Presentation : **MEDI.P-425**

Medicinal Chemistry

Event Hall THU 11:00~13:00

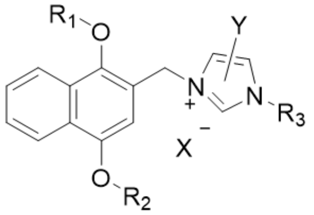
Synthesis of novel 1,4-dialkoxynaphthalen-2-methyl imidazolium salts and its antitumor activity

Haena Lee, Hyejin Moon, Hakwon Kim[1,*]

Chemistry, Kyung Hee University, Korea

[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Imidazole is a 5-membered aromatic heterocyclic compound containing two nitrogen atoms and exhibits various physiological activities. Recently, imidazolium salts have drawn a considerable attention because of their remarkable array of biological activities, especially antitumor activity.In this study, a series of novel 1,4-dialkoxynaphthalen-2-methyl imidazolium salts having various alkoxy groups on the naphthalene ring were designed and synthesized and their antitumor activity was investigated for developing potent antitumor agents.



1,4- dialkoxynaphthalen- 2- methyl imidazolium salts

Poster Presentation : **MEDI.P-426**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis and Biological Activity evaluation of GPR120 selective agonists.

Choi Dami, Sang Jeon Chung[1,*]

Biopharmaceutical Convergence, Sungkyunkwan University, Korea
[1]*College of Pharmacy, SungKyunKwan University, Korea*

G-protein coupled receptor 120 (GPR120) has been emerged as potential drug target for the treatment of type 2 diabetes because its activation is associated with insulin secretion, insulin sensitizing, anti-inflammatory, and fat metabolism. Since, GPR120 agonists have therapeutic potential for anti-diabetes, but few selective agonists have been reported. Herein we describe the design, synthesis, and activity evaluation of novel indole-5-propanoic acid, indole-7-carboxylic acid GPR120 agonist series and conducted SAR studies to optimize GPR120 potency via fischer indole synthesis. Furthermore, we identified compound 2-21, a GPR120 selective agonist, exhibited GSIS and glucagon-like peptide 1 secretory effects. In 3T3-L1 adipocytes, compound 2-21 significantly increase glucose uptake in a concentration-dependent manner. Taken together, this molecule might represent the starting point for the future discovery of GPR120 agonists as antidiabetic drugs.

Poster Presentation : **MEDI.P-427**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis of Some Trazine compounds and agrochemical applications.

Jeong Min Bak, Hee Nam Lim[1,*]

Yeungnam University, Korea

[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

Some functionalized triazine compounds were prepared and evaluated for discovery of the herbicide. To enable acylation of less reactive amines, we adopted sterically less cumbered acylation reagents. The synthesized compounds were evaluated in semi-invivo assay and pots under greenhouse conditions.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MEDI.P-428**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Synthesis of Triazine Derivatives for Discovery of Cellulose Biosynthesis Inhibitors

Chaeyeon Lee, Hee Nam Lim[1,*]

Yeungnam University, Korea
[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

Aminotriazines are privileged scaffold that hold various pharmaceutical and agrochemical activities. We prepared a number of triazine analogs by three different synthetic routes. Those compounds were evaluated in the semi in-vivo assay and the pots in the greenhouse conditions. The synthesis and herbicidal activities are described.

Poster Presentation : **MEDI.P-429**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Development of triple reuptake inhibitor for attention deficit hyperactivity disorder (ADHD)

Ga young Park, Hyeowon Seo, Jieon Lee, Youjeong Choi, Minsoo Song*

New Drug Development Center, Daegu Gyeongbuk Medical Innovation Foundation, Korea

Attention deficit hyperacitivity disorder (ADHD) is a neuropsychiatric disease that is characterized by three core symptoms including inattention, hyperactivity and impulsivity. Current medications for ADHD include stimulants and non-stimulants with methylphenidate (AMP) and amphetamine MPH) as the most widely prescribed drugs. However, their addiction liabilities, therapeutic limitations in comorbid psychiatric diseases, and difficulties for daily life activities due to side effects call for a novel treatment. In this regard, triple reuptake inhibitors (TRI), also known as serotonin-norepinephrin-dopamine reuptake inhibiotr (SNDRI), have emerged as a promising option for the existing ADHD drugs. TRI acts as a reuptake inhibitor of the neurotransmitters serotonin, norepinephrine, and dopamine by inhibiting the serotonin transporter (SERT), norepinephrine transporter (NET), and dopamine transporter (DAT), which results in an increase of neurotransmission.We have developed a novel TRI compound that has comparable in vtiro reuptake inhibitory activity with centanafadine, a competing TRI in Ph 3 clinical trial. In vitro ADME properties were superior to centanafadine, and in vivo DMPK properties were equal to or greater than centanafadine. In vivo efficacy studies using MK-801 mouse model or SHR model revealed that our novel TRI compounds showed significant behavioral efficacies and less side effect potential in dose dependent fashion. Two weeks in vivo toxicity study using SD rat model revealed significantly higher safety potential by showeing TI > 8. Some critical experimental detailes are presented herein.

Poster Presentation : **MEDI.P-430**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Screening for Antifungal Activity of wood plants against Athletes's Foot

Kyoung Tae Lee[*], Jin Sung Huh[1], Su Jin Sim[2], Jaeyoung Hwang[3]

Forest Biomaterials Research center, National Institute of Forest Science, Korea
[1]*Gyeongsang National University, Korea*
[2]*Korea University, Korea*
[3]*Department of Chemistry, Gyeongsang National University, Korea*

This study was performed to investigate and measure the antimicrobial activity of woody species extracts on tidea pedis fungi. To do this, leaves and stems were collected from JinJu, and were used for the extraction with methanol. The experiment was conducted by using the agar diffusion method. The clear zone was measured after incubating the paper disc containing the plant extract in Sabouraud Dextrose medium (SD). The extracts of 142 species of two parts used in this study had inhibitory activity, which confirmed their antifungal activity against tinea pedis [KCTC 6346 (Microsporum audouinii), KCTC 6591 (Microsporum canis), KCTC 6375 (Trichophyton rubrum) and KCTC 6921 (Epidermophyton canis)]. Among them, the extracts of Pyrus pyrifolia (Burm.f.) Naka was showed a zone of inhibition 8.0 ㎜ against Microsporum audouinii (KCTC 6346), while the clear zone of Broussonetia × kazinoki Siebold was 3.0 ㎜ against Microsporum canis (KCTC 6591). In addition, Euonymus japonicus Thunb. showed an effect of 6.0 mm against Trichophyton rubrum (KCTC 6375), and Celastrus orbiculatus Thunb showed an inhibitory line of 10.5 mm against Epidermophyton canis (KCTC 6921), respectively. Therefore, when looking at the effects of the tree extracts on the four kinds of athlete's foot fungus, it was not possible to show the effect on all four kinds, but excellent tree species showing the overlapping effect in the nine kinds such as the Neoshirakia japonica (Siebold & Zucc.) Esser and Pyrus pyrifolia (Burm.f.) Nakai could be selected.

Poster Presentation : **MEDI.P-431**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Neuroprotective effects of 2-heptyl-3-hydroxy-4-quinolone in HT22 mouse hippocampal neuronal cells

Sang Hyuk Lee, Seong-Hee Ko[1], Heesu Lee[1,*], Jae Wook Lee[2,*]

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[1]*College of Dentistry, Gangneung-Wonju National University, Korea*
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The neuroprotective activity of 2-heptyl-3-hydroxy-4(1H)-quinolone (compound 1) was evaluated using theneurotoxicity of glutamate in the HT22 cell line. Compound 1, known as a signal molecule of the bacterialquorum-sensing system, protects neuronal cells from glutamate-induced neurotoxicity by inhibiting cellular Ca2+uptake and glutamate-triggered ROS accumulation. MAPK signaling pathway inhibition by compound 1 wasevaluated by immunoblotting the phosphorylation status of the proteins. Furthermore, pro-apoptotic proteinlevels and AIF translocation to the nucleus were found to be reduced by compound 1. In conclusion, compound 1showed neuroprotective effects by inhibiting apoptotic neuronal cell death.

Poster Presentation : **MEDI.P-432**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Design, Synthesis, and Biological Evaluation of a 2,4-diphenyl-5,6-dihydrobenzo(h)quinolin-8-amine derivative as a novel DNA intercalating topoisomerase II□ poison

Surendra Kunwar, Eung-Seok Lee[1,*]

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Several anticancer agents have been developed and innovative approaches are still ongoing toward cancer type-specific medicines for chemotherapy. As a continuous effort to develop potential chemotherapeutic agents, a novel series of 2,4-diphenyl-5,6- dihydrobenzo(h)quinolin-8-amines containing amino groups, hydroxyphenyl, and fluorine functionalities were designed and synthesized using the one-pot microwave synthesis method. The compounds were evaluated for topo their topo II□ inhibitory and antiproliferative activity against HCT15, and HeLa human cancer cell lines. Among the synthesized thirty compounds, the majority exhibited strong topo II□ inhibition and antiproliferation against the HCT15 colorectal adenocarcinoma cell line. The structure-activity relationship study revealed that compounds with –CF3 and –OCF3 substituents at 4- position and 3’ or 4’-hydroxyphenyl at 2-position attached to the central pyridine ring displayed potent topo II□ and antiproliferative activity in colorectal and cervix cancer cell line. In vitro studies provided evidence that compounds 16, 19, 22, and 28 possess excellent topo II□ inhibition and antiproliferative activity. For a better understanding, topo II□ cleavage complex, EtBr displacement, KI quenching assays, and molecular docking of compound 19 were performed and the results revealed the mode of action as a DNA intercalative topo II□ poison inhibitor. The results obtained from this study provide insight into the DNA binding mechanism of 2,4-diphenyl-5,6-dihydrobenzo(h)quinolin-8-amines and alteration in topo II□ inhibitory and antiproliferative activity with modifications in the rigid structure.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MEDI.P-433**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis and Evaluation of Serinolamide Derivatives as Sphingosine-1-Phosphate-1 (S1P1) Receptor Agonists

Jaehwan Kim, Sun Jun Park[1], Jushin Kim, Yoowon Kim, Elijah Lee, Byungeun Kim[2], Ki Duk Park[3,*]

Korea Institute of Science and Technology, Korea
[1] *Convergence Research Center for Dementia, Division of Bio-Med Science & Technology, Korea*
[2] *Bio-Medical Science & Technology, University of Science and Technology, Korea*
[3] *Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Sphingosine-1-phosphate (S1P) is a sphingolipid metabolite that mediates immune responses by binding to S1P receptors, a group of G protein-coupled-receptors. Sphingosine-1-phosphate receptor 1 (S1P1) plays an important role in regulating the egress of lymphocytes from lymph nodes into the blood circulation. Multiple sclerosis (MS) is an autoimmune disease that affects the central nervous system by autoreactive lymphocytes attacking the myelin sheath. Therefore, reducing the lymphocyte egress is an effective strategy for treating MS. In this study, we developed S1P1 agonists, functional antagonists, that promote S1P1 internalization leading to lymphocyte sequestration in the lymph node. We optimized serinolamide, a marine natural product, synthesis method and synthesized serinolamide derivatives. Compounds **19** and **21** showed good efficacy on S1P1 internalization *in vitro* and peripheral lymphocyte reduction *in vivo*.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MEDI.P-434**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Investigation of the Neuroinflammation Effects of Diosgenin Derivatives

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Research Operations for Brain Science, Korea Institute of Science and Technology, Korea

Diosgenin, a steroidal saponin, is a hydrolyzed product of dioscin produced by the plant family of Dioscoreaceae. Like dioscin, diosgenin, the aglycone of dioscin, shows multiple pharmacological activities such as antitumor, antimicrobial, anti-inflammatory, antioxidative, and tissue-protective properties. Recent studies reported that diosgenin has beneficial in prevention and treatment of neurological diseases such as Alzheimer’s disease, Parkinson’s disease, and neuroinflammation. Its therapeutic mechanisms have been considered as the mediation of signaling pathways like TLR, NF-κB, JNK, and MAPK. Despite of its various pharmacological activities, however, some drawbacks including the poor solubility in aqueous media and indigent bioavailability obstruct its clinical application. Continuing our previous study, here, we broadened the scope of diosgenin derivatives by the introduction of sulfur or nitrogen at the sugar linking oxygen position. All the synthesized compounds were evaluated by CTG and NO assay, which show cytotoxicity and neuroinflammatory effect. Among them, compound 7 shows relatively good neuroinflammatory effect without leading cell death. To confirm its target and role, we are pursuing through biological studies. In addition, the diosgenin derivative having a cholesterol-based structure shows the possibility of being replaced as a component of LNP, a small molecule carrier currently used for mRNA vaccine delivery. By replacing cholesterol with diosgenin derivatives among the components of LNP, anti-inflammatory effects on reactogenicity that occur when mRNA vaccines are administered are expected. Currently, several synthesized diosgenin derivatives have been applied to LNPs and evaluated, and since they showed a level similar to that of naked RNA, it is considered as an alternative component.

Poster Presentation : **MEDI.P-435**

Medicinal Chemistry

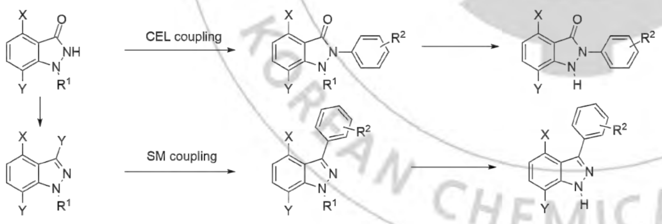
Event Hall THU 11:00~13:00

Synthesis and anti-inflammatory activity of N2-arylindazol-3-one derivatives

<u>Kyungmin Kim</u>, Jeong Ho Kim, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

Indazolone or indazole, a benzene-fused pyrazolone or pyrazole, is an well-known N-heterocycle to exhibit various biological activities. In this study, we synthesized various N2-aryl substituted indazol-3-one derivatives using Chan-Evans-Lam (CEL) coupling reaction of N1-protected N2-unsubstituted indazol-3-one intermediate. Also 3-aryl-substituted indazole derivatives were synthesized using Suzuki-Miyaura (SM) coupling of O-triflate of indazol-3-one derivatives. In addition, their anti-inflammatory activity was investigated.



Poster Presentation : **MEDI.P-436**

Medicinal Chemistry

Event Hall THU 11:00~13:00

CBP/P300 as an important drug target regulated cancer proliferation

Darong Kim*, Yoonna Kwak

Daegu Gyeongbuk Medical Innovation Foundation, Korea

To development the inhibitor of CBP/P300 as anti-cancer drug, we found hit compounds through library screening of in vitro enzyme assay. The treatment of CBP/P300 compounds inhibited cell proliferation in leukemia MV-4-11 cell. Basically, CBP/P300 regulated MYC expression in cancer progression. In mechanism of action (MOA) study, the treatment of CBP/P300 compounds reduced expression of MYC gene. Also, the treatment of CBP/P300 compounds inhibited cell proliferation of liver cancer HepG2 and Hep3B cell and organoid of liver cancer Hep3B cell through inhibiting MYC. In cancer stem cell signaling, CBP/P300 compounds reduced proliferation of cancer stem cell spheroids A2780-SP. Therfore, this work demonstrated that CBP/P300 as an important drug target regulated cancer development.

Poster Presentation : **MEDI.P-437**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis of pyrimidine-core based derivatives as dual EML4-ALK and T790M-mutated EGFR inhibitors

Seungyeon Lee, So Young Kim, Gi Hun Bae, Chunyoung Im*

New Drug Development Center, K-MEDI hub(Daegu Gyeongbuk Medical Innovation Foundation), Korea

Kinase inhibitors, well-known that act selectively on target cancer cell in the treatment of cancer, are widely used as an alternative treatment for chemotherapy, which has side effects. However, there are numerous reports indicate that patients end up gaining drug resistance by using this drug. Epidermal growth factor receptor (EGFR) is well known for the target of the treatment of Non-small cell lung carcinoma (NSCLC). Likewise, although a lot of EGFR inhibitors have been developed, such as Gefitinib, Erlotinib and Afatinib, it has been reported that the prognosis is poor due to drug resistant mutations (eg, T790M). Also EML4-ALK (ALK fusion), anaplastic lymphoma kinase (ALK) gene rearrangement, is target of the NSCLC by ALK fusions. Likewise ALK inhibitors, such as Crizotinib, Ceritinib and Alectinib, has been reported that drug resistance was obsereved. In this study, we report the potent dual EML4-ALK and EGFRT790M inhibitors. we synthesized pyrimidine-core based derivatives targeting EML4-ALK and EGFR T790M. The compounds showed potent in vitro Ba/F3 cellular activity against EML4-ALK, wild type EGFR and T790M-mutated EGFR. Futhermore, the compounds will be optimized to improve ADME, drug properties and selectivity.

Poster Presentation : **MEDI.P-438**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Morphology conserved anatase TiO_2 coated gold nanobipyramids for synergistic photothermal and phothdynamic cancer therapy

Dohyub Jang, Subin Yu[1], Sehoon Kim, Dong Ha Kim[2,*]

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[1]*Ewha Womans University, Korea*
[2]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*

Photodynamic therapy using inorganic materials is recognized as a non-invasive feature and local treatment. However, inorganic photocatalysts have critical threshold in the absorption of high energy photons to introduce in cancer therapy.Meanwhile, plasmonic nanomaterials has drawn attraction due to their tunable localized surface plasmon resonance properties. Particularly, gold nanobipyramids induce much stronger electric fields against gold nanorods commonly used in photothermal therapy. With suitable biocompatibility, plasmonic gold nanomaterials were investigated for cancer treatment and became a promising candidate to redeem the limitations of TiO_2 in biomedical applications. Upon strategic coupling with TiO_2, LSPR-induced hot carriers of plasmonic Au nanomaterials are injected into the conduction band of TiO_2 over the Schottky barrier, which can generate reactive oxygen species. Despite of these advantages, Au NBP is hard to utilized due to their low thermal stability. Herein, we newly developed anatase TiO_2 caoted Au NBP (Au NBP/a-TiO_2) as a novel metal/semiconductor heterostructure for NIR-responsive phototherapy. LSPR-derived hot electrons generated by NIR light were injected into the conduction band of the anatase TiO_2 nanoclusters, inducing the reduction of oxygen to super oxide and finally producing ·OH radical species. Simultaneously, the LSPR-induced photothermal effect was investigated for photothermal therapy. The Au NBP/a-TiO_2 capable of ROS and heat generation by NIR light is promising as effective cancer theranostic nanoplatforms for synergistic photodynamic and photothermal therapy.

Poster Presentation : **MEDI.P-439**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Copper complex of a thienyl-hydrazone rhodamine derivative is a highly selective colorimetric sensor for pyrophosphate

Pradeep Kumar, Young Jun Seo[1,*]

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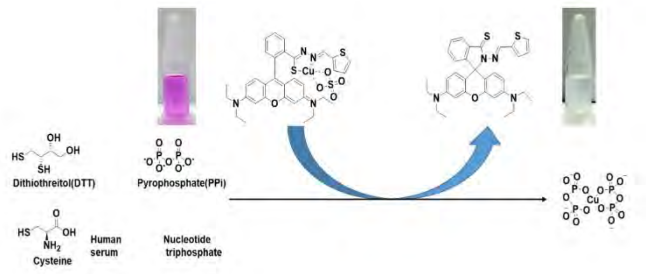
[1]*Department of Chemistry, Jeonbuk National University, Korea*

Detection of pyrophosphate (PPi) can be used to monitor gene replication, transcription, and other forms of enzymatic DNA/RNA synthesis, In this study we prepared a copper complex-1 that could detect PPi specifically and selectively in the presence of other anions and biological molecules. copper complex-1 exhibited its highly selective PPi sensing capability when applied to rolling circle amplification and in vitro transcription in samples containing high concentrations of DTT, making it a promising candidate for colorimetric detection of RNA/DNA when using amplification techniques



Poster Presentation : **MEDI.P-440**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Figure out the systematic pathway of cytoplasmic antibiotic delivery using simple bidentate siderophore mimetics

Do Young Kim, Heeyeong Lee, Hak Joong Kim[1,*]

Chemistry, Korea University, Korea

[1]*Department of Chemistry, Korea University, Korea*

Humans are devising various methods for therapeutic conquest of gram-negative bacteria, but in order to overcome antibiotic resistance due to the cell permeability problem of antibiotics, sideromycin using siderophore as a bacterial membrane transporter is the most efficient solution. Among them, cefiderocol, which was approved by the FDA in 2019, showed high antibacterial activity against various types of gram-negative bacteria and proved the efficiency of sideromycin. However, it has a limitation that it is limited to the periplasmic delivery of antibiotic. In fact, although a significant number of cytoplasmic antibiotics have low antibacterial activity against gram-negative bacteria due to cell membrane permeability problems, there are few examples is reported that antibacterial activity is not significantly different from that of treating cytoplasmic antibiotics only. Thus, systematic details how to cytoplasmic sideromycins can be delivered to cytoplasm is necessary for effective sideromycin design. In this study, synthesized 20 simple bidentate sideromycins, conjugate with trimethoprim, which is a cytoplasmic antibiotic, and conducted the antibacterial activity check as MIC assay for figure out the pathways which they transfer trimethoprim to cytoplasm. The MIC assay was conducted not only *escherichia coli* WT, but also mutant strains which are protein, involved in intracellular active transport of siderophore, knockout strains were used, and conducted PAMPA assay to evaluate the cell membrane passive diffusion capability of sideromycin. Clarifying the cytoplasmic antibiotic delivery pathway of simple bidentate sideromycins through these studies may further reinforce the influence of sideromycin on overcoming antibiotic resistance of gram-negative bacteria.

Poster Presentation : **MEDI.P-441**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Development of new target protein catalyst compounds as a novel class of H_2O_2 scavenger for treatment of Alzheimer’s Disease

Elijah Lee, **Ki Duk Park**[1,*]

Convergence Research Center for Diagnosis, Treatment and Care System of Dementia, United States

[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Alzheimer’s disease (AD) is the most common form of dementia and is a progressive neurodegenerative disease characterized by memory loss. In the AD brain, reactive oxygen species (ROS) levels are significantly higher than that of healthy aging brain. Hydrogen peroxide (H_2O_2) is a representative ROS that causes oxidative stress and is a product of many different metabolic pathways in AD. We recently investigated the mechanism of action of the drug AAD-2004, which is effective in scavenging H_2O_2 in neurodegenerative disease mouse model. In this study, we aim to optimize the efficacy and drug-like properties of AAD-2004 to develop a novel H_2O_2 target candidate for treatment of AD. We synthesized 33 novel compounds and evaluated the H_2O_2 scavenging activity using an optimized in vitro assay system. Among them, KDS12025 exhibited five times the efficacy of AAD-2004 (EC_{50}: 0.199 µM to 0.99 µM, respectively) and also showed favorable microsomal stability (57.6% in human during 30 min to

Poster Presentation : **MEDI.P-442**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Discovery of Novel Sphingosine-1-Phosphate-1 ($S1P_1$) Receptor Agonists for the Treatment of Multiple Sclerosis

Yoowon Kim, Ki Duk Park*

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea

The sphingosine-1-phosphate-1 ($S1P_1$) receptor agonists have great potential to treat multiple sclerosis (MS) because they can inhibit lymphocyte egress through receptor internalization. We designed and synthesized triazole and isoxazoline derivatives to discover a novel $S1P_1$ agonist for MS treatment. Of the two scaffolds, the isoxazoline derivative was determined to have excellent in vitro efficacy and drug-like properties. Among them, compound **21l** was found to have superior drug-like properties as well as excellent in vitro efficacies (EC_{50} = 7.03 nM in β-arrestin recruitment; EC_{50} = 11.8 nM in internalization). We also confirmed that **21l** effectively inhibited lymphocyte egress in the peripheral lymphocyte count (PLC) test and significantly improved the clinical score in the experimental autoimmune encephalitis (EAE) MS mouse model.

Poster Presentation : **MEDI.P-443**

Medicinal Chemistry

Event Hall THU 11:00~13:00

[Withdrawal] TNBC cell-specific codelivery of erlotinib and doxorubicin using PEG-cleavable and cell penetrating peptide-exposable nanoliposomes

Chami Park, Ji Hye Choi[1], Sujin Kim, Hasoo Seong[2,*]

Eco-Friendly New Materials Research Center , Korea Research Institute of Chemical Technology, Korea

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[2]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

- Withdrawal -

Poster Presentation : **MEDI.P-444**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Synthesis and evaluation of novel series of vinyl sulfone derivatives from Veda-1209 as promising Nrf2 activators for alleviating neuroinflammation

Byungeun Kim, Ki Duk Park*

Convergence Research Center for Brain Science, Korea Institute of Science and Technology, Korea

Accumulated oxidative damage is related to neurodegenerative condition. Indeed, decrease of expression of the nuclear factor E2-related factor 2 (Nrf2) have been reported in Alzheimer's disease patient's brain. Nrf2-antioxidant responsive element signaling is the main pathway responsible for cellular defense system against oxidative or electrophilic stress. Nrf2 plays a vital role in anti-inflammatory responses as well as antioxidant defenses by mediating the expression of various antioxidant enzyme genes and pro-inflammatory cytokines. So Nrf2 activation has emerged as a therapeutic target for neurodegenerative diseases. Several studies have reported that chalcone consisting of α,β-unsaturated carbonyl system exhibits several biological activities including anticancer, antioxidant, antibacterial and anti-inflammatory properties. Veda-1209, a chalcone derivative, is Nrf2 activator currently undergoing preclinical testing for the treatment of various diseases. In this work, a series of novel Veda-1209 derivatives were synthesized by substituting vinyl sulfone and screened for their Nrf2 activating efficacy, antioxidant and anti-inflammatory effects in vitro. Among the synthesized compounds, a potent compound (6e) showed superior Nrf2 activation compared to Veda-1209 (Nrf2 activation EC50: Veda-1209 = 625 nM vs compound 6e = 38 nM). Unlike insufficient drug-like properties of Veda-1209, 6e exhibited better drug-like properties including stability and CYP enzyme interaction. Furthermore, compound 6e induced the expression of the Nrf2-dependent enzymes at protein levels and suppressed the induction of pro-inflammatory effects. To further validate potency of 6e as an Nrf2 activator, we checked memory impairment recovery in a scopolamine-induced mouse model.

Poster Presentation : **MEDI.P-445**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Progress in discovery of a VHL-ligand based Hsp90-selective degrader

Jimin Park, Do Young Kim, Hak Joong Kim*

Department of Chemistry, Korea University, Korea

Hsp90 is a protein expressed to reduce cellular damage under cell stress and is a molecular chaperone involved in the stability and function of proteins. Since Hsp90 is particularly associated with tumor cell survival, many studied have been conducted to inhibit its chaperone activity. However, no studies have passed clinical trials, due to cellular toxicity and inefficiency. Therefore, to overcome these issues, a degradation approach was attempted through PROTAC Molecule.Proteolysis targeting chimera (PROTAC) is a molecule that can selectively degrade protein of interest (POI) and is composed of ligands for POI and a E3 ligase conjugated with each other via covalent linker. This can be effectively used to degrade specific proteins, so CRBN-based PROTACs with Hsp90 as targets have been recently reported. We are conducting research focusing on VHL-base Hsp90 PROTAC, and this poster presents our recent progress in synthesis, *in vitro* evaluation of various PROTAC compounds targeting Hsp90.

Poster Presentation : **MEDI.P-446**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Korea Bio Data Station(K-BDS) Hardware System Support Program for Bio Research Data Utilization

Jung Woo Park

Center for Supercomputing Applications, Korea Institute of Science and Technology Information, Korea

With the goal of establishing a data-based bio research environment at the national level, 'National Bio Data Station (K-BDS)', a bio data platform construction project that integrates, collects, and provides bio data dispersed by department/project/researcher, started in 2021. KISTI and KRIBB Participated in this project. KISTI has established analysis hardware system resources to promote the use of national biodata and to strengthen national bio-field research and industrial competitiveness. We are operating the 'Biodata Analysis Infrastructure Utilization Support Program', which provides domestic researchers with infrastructure system resources built to promote domestic bio/new drug-related big data analysis and artificial intelligence research.The target of support is all researchers from domestic companies, research institutes, universities, public institutions, hospitals, etc. that conduct research in the field of bio/new drugs, and supports the calculation and storage resources and development environment of the analysis system. The target of support is all researchers from domestic companies, research institutes, universities, public institutions, and hospitals conducting research in the field of bio/new drugs.

Poster Presentation : **MEDI.P-447**

Medicinal Chemistry

Event Hall THU 11:00~13:00

Central administration of afzelin extracted from Ribes fasciculatum improves cognitive and memory function in AD models

Min Soo Kim*, Chun Whan Choi[1]

Brain Science Institute, Korea Institute of Science and Technology, Korea
[1]*Natural Product Research Team,, Gyeonggi Biocenter, Korea*

Neurodegenerative disorders are characterized by the decline of cognitive function and the progressive loss of memory. The dysfunctions of the cognitive and memory system are closely related to the decreases in brain-derived neurotrophic factor (BDNF) and cAMP response element-binding protein (CREB) signalings. Ribes fasciculatum, a medicinal plant grown in diverse countries, has been reported to pharmacological effects for autoimmune diseases and aging recently. Here we found that afzelin is a major compound in Ribes fasciculatum. To further examine its neuroprotective effect, the afzelin (100 ng/μl, three times a week) was administered into the third ventricle of the hypothalamus of C57BL/6 mice for one month and scopolamine was injected (i.p.) to these mice to impair cognition and memory before each behavior experiment. The electrophysiology to measure long-term potentiation and behavior tests for cognitive and memory functions were performed followed by investigating related molecular signaling pathways. Chronic administration of afzelin into the brain ameliorated synaptic plasticity and cognitive/memory behaviors in mice given scopolamine. Studies of mice’s hippocampi revealed that the response of afzelin was accountable for the restoration of the cholinergic systems and molecular signal transduction via CREB-BDNF pathways. In conclusion, the central administration of afzelin leads to improved neurocognitive and neuroprotective effects on synaptic plasticity and behaviors partly through the increase in CREB-BDNF signaling.

Poster Presentation : **MEDI.P-448**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Anti-inflammatory Effect of Phloroglucinol Derivatives Attenuates Cognitive Impairment in a LPS-Induced Mouse Model

Jushin Kim, Ki Duk Park*

Convergence Research Center for Brain Science, Korea Institute of Science and Technology, Korea

Neuroinflammation is an inflammatory immune response that occurs in the central nerve system. It is one of the important causes in neurodegenerative diseases, such as Alzheimer's disease and Parkinson's disease. Phloroglucinol (PG) is a natural product from brown algae and has been reported to have an anti-inflammatory effect. In this study, we synthesized PG derivatives to enhance the anti-inflammatory activities. Among the PG derivatives, KDS4156 suppressed the production of inflammatory molecule nitric oxide (NO) more effectively than PG. Furthermore, KDS4156 concentration-dependently reduced expression of pro-inflammatory cytokines such as TNF-α, IL-6, IL-1β and NO producing enzyme iNOS in the LPS-stimulated BV-2 microglial cells. We also confirmed thatKDS4156 did not exhibit significant cytotoxic activity compared to PG. Finally, KDS4156 alleviated cognitive impairment and glial activation in LPS-induced mouse model. These findings suggest that a novel PG derivative,KDS4156, could be a potential treatment for neurodegenerative diseases.

Poster Presentation : **MEDI.P-449**
Medicinal Chemistry
Event Hall THU 11:00~13:00

Type 2 Diabetes Mellitus Treatment with Gene Delivery System

Jeongman An, Yong-kyu Lee[1,*]

Department of Bio Engineering, Hanyang University, Korea
[1]*Department of Chemical and Biological Engineering, Korea National University of Transportation, Korea*

We investigated the effect of dose quantity on the therapeutic efficacy of oral GLP1 gene therapy. Using a multimodal gene complex (GLP1/PTCA), we showed glycemic improvement drawn for up to 1 week in three progressives diabetic mouse models. To the best of our knowledge, this is the first report of any dosage form of GLP1 agonist for the most extended period of glucose control using a minimal quantity of genes (＜0.5 mg human equivalent dose). Since Rybelsus® is the only FDA-approved oral GLP1 agonist that needs to be taken with 7 or 14 mg daily, oral GLP1/PTCA may provide the first once or bi-monthly oral treatment option for diabetic patients according to allometric principles.

Poster Presentation : **MAT.P-450**

Material Chemistry

Event Hall THU 11:00~13:00

Electric polarization and ferroelectricity on a antiferromagnet triangular lattice, RbFe(MoO4)2

Changhoon Lee[*], **Ina Park**[1], **Taesu Park**[1], **Ji Hoon Shim**[1,*]

Center for Complex Phase of Materials, Max Planck/ POSTECH , Korea

[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

RbFe(MoO4)2 is a rare example of a nearly two-dimensional Heisenberg antiferromagnet on a triangular lattice. RbFe(MoO4)2 belongs to the family of layered trigonal molybdates and tungstates with the structure of KAl(MoO4)2 type.. The space group of RbFe(MoO4)2 at room temperature is $P\bar{3}m1$. However, the RbFe(MoO4)2 exhibits structural phase transition at around 190K from $P\bar{3}m1$ to $P\bar{3}1$. On the basis of density functional theory calculations, we explored the origin of the observed spin frustrated magnetic structure of RbFe(MoO4)2 by evaluating its spin exchange interactions to find that spin exchanges are frustrated within triangular lattice (//ab) but also between layers (//c). Our analysis predicts that triangular lattice is a multiferroic with a ferroelectric polarization of ~10 μC/m2 along c-direction, and a field-induced reversal of the ferroelectric polarization of RbFe(MoO4)2 can occur by changing of C3 rotational axis center in triangular lattice. We were also investigated change of electronic structure as a change of polarization direction of RbFe(MoO4)2.

Poster Presentation : **MAT.P-451**

Material Chemistry

Event Hall THU 11:00~13:00

Gas Encapsulating Layer for Stretchable Electronics by Selective Infiltration of Al2O3 in Polymer Films

Sangho Cho*, **Myong Mo Sung**[1,*]

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[1]*Department of Chemistry, Hanyang University, Korea*

Atomic layer infiltration (ALI) has been performed for the preparation of Al2O3-polymer hybrid layer as thin gas barrier films. Filling of the free volumes of polymers at the subsurface region with Al2O3 resulted in an excellent water vapor transmission rate (WVTR) low enough to be used as gas encapsulating films for display applications. Among various polymeric substrates, PET, PI, and Nylon 6 formed hybrid thins layers with the infiltration depth in the nanometer ranges while Al2O3 could not infiltrate into PFA and PS films. The selectivity of Al2O3 infiltration into polymer films was employed to prepare stretchable gas encapsulating films by encapsulating individual segments of 144 Ca dots by Al2O3-PET hybrid films on PFA polymer substrate. Regardless of bending and stretching, it exhibited extremely low gas barrier properties with WVTR of

Poster Presentation : **MAT.P-452**

Material Chemistry

Event Hall THU 11:00~13:00

Nanoadsorbent-embedded hybrid filters for elimination of anionic surfactants

JiHee Choi, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Surfactants discharged from domestic sewage and factory wastewater interfere with the growth of aquatic organisms and are well absorbed and accumulated in the human body, acting as a potential carcinogen. Therefore, immediate removal of surfactants is important to humans and the environment. Hollow nano/micro adsorbents can be used as high-performance adsorbents due to their high specific surface area to volume ratio. However, there is a risk of leakage with nano/micro materials. We report a novel adsorption filter containing a hollow nano/micro-adsorbent that reduces the risk of leakage and has a high adsorption capacity.

Poster Presentation : **MAT.P-453**
Material Chemistry
Event Hall THU 11:00~13:00

A flexible sponge filter loaded with nanocatalysts for reductive decomposition of organic pollutants

HeeJu Kim, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Water pollution by heavy metals, organic dyes, and oily wastewaters has become a serious environment issue. Diverse technologies have been developed to address this issue. Among these methods, metal nanocatalysts have been extensively used for synthesis of organic materials and decomposition/conversion of organic pollutants due to their excellent catalytic activity and high specific surface area. However, it has been recently reported that unintended leakage of nanocatalysts (nano-sized particles/structures) into the environment can cause a significant threat to the environment and public health. Thus, it is needed to develop a novel catalytic filter that does not have a risk of leakage, has a rapid catalytic reaction, high flux, easy increase/decrease in the amount of catalyst, and excellent reusability.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-454**

Material Chemistry

Event Hall THU 11:00~13:00

A novel photothermal purification of wastewaters through water evaporation

Su Hyeon Son, Won san Choi*

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Wastewaters emitted from various industries have become a serious environmental issue and problem. Desalination of seawater or wastewater is considered a reliable solution for the challenges of water scarcity and the pollution of marine eco-system. We report photothermal evaporator/adsorbents with hydrophilic and hydrophobic natures for water evaporation and purification.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-455**

Material Chemistry

Event Hall THU 11:00~13:00

A strategy for reducing viscosity and enhancing absorption capacity of crude oil

Youngju Jung, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Various methods including combustion and chemical dispersants have been reported for cleanup of crude oil. However, these methods require a huge consumption of energy resources and time and cause environmental pollution as well. Thus, development of functional absorbents is essential for effective and fast cleanup of crude oil in the sea because the viscosity of crude oil increases as the temperature of seawater decreases, leading to the severe fouling of absorbent. We report photothermal absorbent balls that have a large specific surface area and are effective in reducing the viscosity of crude oil.

Poster Presentation : **MAT.P-456**

Material Chemistry

Event Hall THU 11:00~13:00

Polymer membranes with anti-oil-fouling characteristics for cleanup of crude oil at low temperature

Yujin Seo, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Frequent oil spill accidents can cause great environmental problems. Various approaches have been proposed to introduce hydrophilic nature and roughness in hydrophobic membranes. However, membrane fouling may still occur due to the incomplete coverage of hydrophobic membranes by hydrophilic materials. To address this issue, we report a superhydrophilic and underwater superoleophobic membrane that is robust, fouling-resistant, and synthesized by easy scale-up method.

Poster Presentation : **MAT.P-457**

Material Chemistry

Event Hall THU 11:00~13:00

Topotactic Reaction of Lithium by Thermally Decomposed Lithium Aluminum - Layered Double Hydroxides

Yongju Lee, Duk-Young Jung*

Department of Chemistry, Sungkyunkwan University, Korea

To adsorb and collect lithium in aqueous media, lithium aluminum layered double hydroxide (LiAl2-LDH) nanocrystals on aluminum metal substrates were synthesized, which is transformed above 250 oC into a mixture of LiCl and Li-Al-O-OH and dissolved lithium of 85 % in deionized water at 25 oC. Amorphous Li-Al-O-OH residues on the aluminum metal substrate were capable of adsorbing lithium ions back to LiAl2-LDH phase. Thermal treatment followed by additional lithium intercalation suggested a topotactic reaction of lithium ions between amorphous Li-Al-O-OH and LiAl2-LDH. We also proposed a facile recycling method of lithium ions by peeling off the Li-Al-O-OH layer to adsorb lithium ions on aluminum metal substrate again.

Poster Presentation : **MAT.P-458**

Material Chemistry

Event Hall THU 11:00~13:00

Crown-Ether Functionalized Naphthalene Derivatives for Fluorescent Lithium Sensors

Haneul Kim, Sumin Lee, Soyeon Kim, Byungjin Koo[*]

Department of Polymer Science and Engineering, Dankook University, Korea

Detection and quantification of lithium ions are of critical importance for lithium-ion battery recycling and lithium extraction from lithium resources. In this work, we report the synthesis of lithium-detecting small molecules that could selectively detect lithium ions. Naphthalene monoimide, which was used as a fluorophore, was modified with 1-aza-12-crown-4 through a Buchwald-Hartwig amination reaction. This molecule was characterized by 1H NMR and LC-MS. This naphthalene derivative possesses a donor-fluorophore-acceptor structure, indicating that the initial fluorescence in the absence of lithium ions was quenched owing to the electron transfer from the crown moiety serving as a donor. Upon the addition of lithium ions in organic solvents, we observed the fluorescence increase due to the lithium binding to the donor that would prevent electron transfer. We are currently investigating other cations (Na^+ and K^+) to confirm the selectivity as well as synthesizing similar naphthalene derivatives to improve sensitivity of this fluorescent lithium sensors.

Poster Presentation : **MAT.P-459**

Material Chemistry

Event Hall THU 11:00~13:00

Implementation of a portable aquatic toxin detection device using large-diameter carbon nanotubes attached with gold particles

Songmi Bae, Don Kim*

Department of Chemistry, Pukyong National University, Korea

We prepared graphitized carbon nanotubes (CNTs) prepared through thermal conversion of polyvinylpyridone (PVP) and sucrose based on an anodized aluminum oxide (AAO) template. Au nanoparticles (AuNPs) attached CNTs. The synthesis of Au-CNTs was confirmed by SEM, XRD, Raman, TEM, and the like. A top gate type FET sensor was combined using activated Au-CNT, and the CNT sensor was extended to the detection area of a biological sample using an aptamer with high selectivity. The S-(active element)-D shape of the field effect transistor (FET) was completed by fixing the bioactivated MCTA-MWCNT to the Au interdigitated electrode. When placed in the sample solution between the S and D electrodes and immersed in the Ag/AgCl-like reference electrode, it becomes the gate (G) electrode and the top gated FET is completed. The sensor sensitivity = 1.09 (ng/mL)-1, the detection limit = 0.25 ng/mL and it could assay MC-LR level in freshwater within the world health organization guideline (≤ 1.0 ng/mL)

Poster Presentation : **MAT.P-460**

Material Chemistry

Event Hall THU 11:00~13:00

Holey Titanium Nitride Nanosheet as an Efficient Hybridization Matrix for Enhancing the Supercapacitor Performance of Layered Double Hydroxide

Yeon Hu Park, Xiaoyan Jin, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

Hybridization with conductive species has garnered significant research interest as an effective route to explore high-performance materials. In this study, an efficient synthetic route to high-performance supercapacitor electrode is developed by employing conductive holey TiN nanosheet (NS) with coordinatively unsaturated sites as a hybridization matrix. The strongly-coupled nanohybrids of layered double hydroxide (LDH)-holey TiN can be synthesized by the crystal growth of Ni-Fe-LDH NSs on the surface of holey TiN NSs. In the obtained nanohybrids, Ni-Fe-LDH NSs are homogeneously immobilized on the surface of holey TiN NSs without significant agglomeration. The obtained Ni-Fe-LDH-TiN nanohybrid shows excellent supercapacitor performance, highlighting the merit of holey TiN as a hybridization matrix for Ni-Fe-LDH. The beneficial effect of holey TiN NS incorporation on the electrode performance of Ni-Fe-LDH NS is attributable to the improved charge transfer kinetics, increased porosity, and the increase of surface electrophilicity. The present study underscores that defective holey TiN NS can act as an effective hybridization matrix for LDH NS to explore novel multifunctional hybrid materials for electrodes.

Poster Presentation : **MAT.P-461**

Material Chemistry

Event Hall THU 11:00~13:00

An Efficient Synthetic Route to Carbon-Coated Metal/Metal Oxide with Promising Electrocatalytic Activity toward Hydrogen Evolution Reaction

So Yeon Yun, Xiaoyan Jin*, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

In this study, a novel one-pot carbon-coating-ex-solution synthetic route to high performance hydrogen evolution reaction (HER) electrocatalyst is developed by the carbon coating for Ru substituted MnO_2 nanowires at 500 ℃ in the C_2H_2 atmosphere. The reaction of C_2H_2 with $Mn_{1-x}Ru_xO_2$ nanowires induces the phase transition to carbon coated-Ru clusters/MnO nanocomposite. The obtained carbon@Ru-MnO exhibits much higher HER electrocatalytic activity than do the pristine $Mn_{1-x}Ru_xO_2$ nanowires and Ru free-carbon@MnO materials, highlighting the beneficial role of the carbon-coating-ex-solution route and Ru substitution. The beneficial effect of simultaneous carbon coating/ex-solution process on the HER electrocatalytic activity is attributable to the improved charge transfer kinetics, increased porosity, and the increase of electrocatalytic kinetics. The present study underscores that the combinative carbon-coating-ex-solution synthetic strategy can provide an effective means to explore efficient composite electrocatalyst materials.

Poster Presentation : **MAT.P-462**
Material Chemistry
Event Hall THU 11:00~13:00

Sub-10 μm Resolution of Micropatterned Copper Nanowire Electrodes by Reverse Offset Printing

Jongyoun Kim, Youngu Lee[1,*]

Enegy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Copper nanowires (CuNWs) possess key characteristics for realizing flexible transparent electronics. High-quality CuNW micropatterns with high resolution and uniform thickness are required to realize integrated transparent electronic devices. However, patterning high-aspect-ratio CuNWs is challenging because of their long length, exceeding the target pattern dimension. This work reports a novel reverse offset printing technology that enables sub-10 μm high-resolution micropatterning of CuNW transparent conducting electrodes (TCEs). The CuNW ink for reverse offset printing was formulated to control viscoelasticity, cohesive force, and adhesion by adjusting the ligand, solvents, surface energy modifiers, and leveling additives. An inexpensive commercial adhesive hand-roller achieved a simple, fast, and scalable micropatterning of CuNW TCEs. Easy production of high-quality CuNW micropatterns with various curvatures and shapes was possible, regardless of the printing direction. The reverse offset-printed CuNW micropatterns exhibited a minimum of 7 μm line width, and excellent pattern qualities such as fine line spacing, sharp edge definition, and outstanding pattern uniformity. In addition, they exhibited excellent sheet resistance, high optical transparency, outstanding mechanical durability, and long-term stability. Flexible light-emitting diode circuits, transparent heaters, and organic light-emitting diodes can be fabricated using high-resolution reverse offset-printed CuNW micropatterns for applications in flexible transparent electronic devices.

Poster Presentation : **MAT.P-463**

Material Chemistry

Event Hall THU 11:00~13:00

A study on crystallization of high-purity lithium carbonate by developing a process for removing impurities from low-grade lithium waste liquid

Sechul Hong

Test Analysis Research Center, Gumi Electronics & Information Technology Research, Korea

As continuous demand for electric vehicle batteries is expected, countries around the world are making efforts to secure lithium. In the case of Korea, where lithium is not abundant, all lithium needed for industry is imported from abroad. In addition, various efforts are being made to secure lithium due to an increase in lithium demand and an increase in import prices. Lithium carbonate recovered from the waste solution generated during the lithium secondary battery manufacturing process contains heavy metals such as cobalt, nickel, and manganese. In this study, the low-grade lithium waste liquid generated after the NMC recovery process in the waste lithium secondary battery was used. In order to remove impurities contained in the low-grade lithium waste liquid, more than 95% of heavy metals were removed by selecting the leaching solvent and optimal conditions such as concentration, pH, and reaction time. For crystallization of lithium carbonate, it was recrystallized by reacting with an aqueous sodium carbonate solution in a lithium carbonate solution from which solid impurities were removed by leaching lower lithium carbonate by pH. Based on the lithium content in the lithium carbonate solution, 1.5 M aqueous sodium carbonate solution was added as 1 equivalent of sodium carbonate to crystallize lithium carbonate powder. Crystallized lithium carbonate was confirmed by XRD.

Poster Presentation : **MAT.P-464**

Material Chemistry

Event Hall THU 11:00~13:00

Properties of CuAg foil consisting of CuAg/Ag nano-multilayers prepared via pulse electrodeposition in methanesulfonate-based solution.

Wonhyo Kong, Seunghoe Choe*

Electrochemistry department, Korea Institute of Materials Science, Korea

CuAg alloy is an attractive material for various applications such as semiconductor probe cards, slip ring brushes, and low-voltage electrical contacts because of its high conductivity (>70%IACS) and high strength (>1 GPa). Recently, the thinning of CuAg foils below 100 um is highly required due to the miniaturization of electronic devices, but it is difficult to obtain thin CuAg foil via the conventional deformation process. Nanocrystalline CuAg foils prepared by the electrodeposition method is a promising material that satisfies high strength, high conductivity, and low thickness, but the denseness of the deposition layer, the toxicity of the solution, and the thermal stability of the formed nanostructure are still regarded as problems. In this study, CuAg foils with a CuAg/Ag multilayered structure was fabricated by pulse electroplating in an environmentally friendly methanesulfonate(MSA)-based solution, and their properties were evaluated. As-deposited CuAg/Ag foil with an interlayer distance of 9 nm exhibited high strength (927 MPa), high conductivity (67%IACS), and good thermal stability. Annealing at mild condition further improved the strength (1 GPa) and conductivity (74%IACS) because of Ag segregation-induced grain boundary stabilization.

Poster Presentation : **MAT.P-465**

Material Chemistry

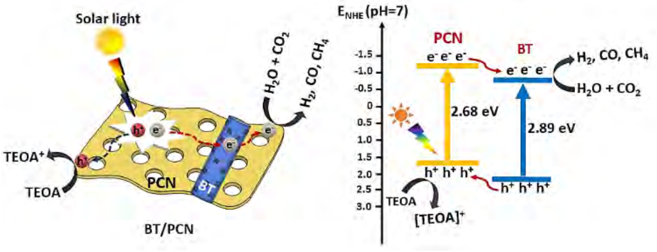
Event Hall THU 11:00~13:00

Nanocavity-assisted Single-Crystalline Ti^{3+} Self-Doped Blue TiO_2(B) as Efficient Cocatalyst for High Selective CO_2 Photoreduction of g-C_3N_4

Praveen kumar Dharani, **Tae Kyu Kim**[*]

Department of Chemistry, Yonsei University, Korea

Two-dimensional (2D) graphitic carbon nitride (g-C_3N_4) has invoked significant interest for photocatalytic applications for its excellent features such as high surface area, visible light absorption, and easy transportation of photogenerated charge carriers, but the most reported g-C_3N_4 show relatively low photoactivity due to inferior conductivity and rapid recombination of carriers. These can be overcome by inducing porosity in g-C_3N_4, followed by exfoliation and combining with other materials. Herein, we synthesize nanocavity-assisted oxygen deficient Ti^{3+} self-doped blue TiO2(B) nanorods (BT) and integrated on exfoliated porous g-C_3N_4 (PCN). The synthesized materials are tested for photocatalytic conversion of CO_2 into solar fuels (H_2, CO, and CH_4). The fabricated BT/PCN heterostructures exhibit higher photocatalytic CO_2 conversion activity and 92% CO-evolving selectivity than BT and PCN. The enhancement in activity of BT/PCN can be attributed to the efficient separation and transportation of charge carriers, facilitated by the unique properties of BT, PCN, and their synergistic interactions. We believe that these results can contribute to the improvement of cost-effectiveness, feasibility, and overall performance for real photocatalytic systems



Poster Presentation : **MAT.P-466**

Material Chemistry

Event Hall THU 11:00~13:00

Rotation of graphene by edge state engineering for stacking angle-controlled bilayer graphene on Cu(111) surface

Hyeyeon Cho, Hee Cheul Choi[1,*]

Chemistry, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Comprehensive understanding of bilayer graphene (BLG) growth with desired stacking angle by chemical vapor deposition (CVD) is an uprising issue because of the stacking angle-dependent properties. Here, we report rotation behavior of graphene layer through edge state engineering induced by controlling growth temperature. We found the rotation behavior of graphene layer through observing the decreased population of AB-stacking form during the BLG growth. Using rotation phenomenon, highly selective growth of AB-stacked BLG (90.4 %) and 30°-twisted BLG (57.5 %) was achieved compared to conventional CVD method by controlling the interaction between the graphene layer and Cu(111) catalyst surface. To obtain the selectivity, the rotation of graphene layer is blocked or accelerated via descending or ascending growth temperature, respectively. We provide both experimental and computational evidence of rotation and selective growth of BLG with desired stacking angle. Our results demonstrate the motion of graphene and the stacking angle-control technique during the CVD process.

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Poster Presentation : **MAT.P-467**

Material Chemistry

Event Hall THU 11:00~13:00

Redox-triggered highly conducting cocrystals

Hye Soo Kim, Hee Cheul Choi[1,*]

Division of Advanced Materials Science, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Since the emergence of tetrathiafulvalene-7,7,8,8-Tetracyanoquinodimethane (TCNQ) charge transfer (CT) complex exhibiting remarkably high electrical conductivity, various cocrystals of TCNQ have been reported. Despite the superior property of TCNQ as a CT complex component, not all TCNQ compounds exhibit such a high electrical conductivity mainly because of the insufficient charge transfer due to the inadequate redox potential between donors and TCNQ. Here, we present a general approach to making highly conducting systems by using TCNQ as a cocrystal component and selectively reducing TCNQ to induce electron doping effect. As an example, highly conducting fluoranthene (FA)-TCNQ cocrystal is prepared by reducing TCNQ with hydrazine vapor. This approach is confirmed to be versatile for various polycyclic aromatic hydrocarbon (PAH) molecules; Anthracene-TCNQ and Coronene-TCNQ cocrystals. In this presentation, details about the synthesis of FA-TCNQ cocrystal, selective doping, and the origin of the conductivity increase will be discussed.

Poster Presentation : **MAT.P-468**

Material Chemistry

Event Hall THU 11:00~13:00

Comparative study for inclusion phenomena of BP-5 into the interlayer space of LYH and LDH

Yoonjae Choi, Se-Young Cho, Song-ho Byeon[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

The sunscreening agent, 2-hydroxy-4-methoxybenzophenone-5-sulfonic acid (Benzophenone-4; BP-4), along with its sodium salt (BP-5), is commercially used to protect the skin from damage by a majority of UV radiation from the sunlight. However, BP-4 has been found to induce cosmetic dermatitis of the face and neck and also causes sensitization at other locations. Furthermore, owing to its widespread and continuing use and release into aquatic environments, BP-4 has become an emerging pollutant. For this purpose, layered host matrices comprising inorganic ions interchangeable with organic ions are particularly of interest because guest organic molecules can be readily stored by an exchange reaction, protected in the interlayer space from aging by heat, UV light, and oxygen. Layered double hydroxides (LDHs) and layered rare-earth hydroxides (LRHs) are recently considered as candidate materials to prevent the penetration of the skin by BP4 or BP5 anions as well as release of BP4 or BP5 anions into aquatic systems. In this work, ZnAl-LDH (Zn2/3Al1/3(OH)2(NO3)1/3·nH2O) and LYH (Y2(OH)5NO3·nH2O) were compared as inorganic hosts for BP-5 anion. Interlayer arrange and release behavior, UV-filtering performance, and photostability of BP-5 anions were compared in these two inorganic host materials.

Poster Presentation : **MAT.P-469**

Material Chemistry

Event Hall THU 11:00~13:00

Tyrosinase inhibition effect of kojic acid intercalated into the gallery of layered yttriumhydroxide

Myeongjin Kang, Yoodong Chang, Song-ho Byeon[1,*]

Applied Chemistry, Kyung Hee University, Korea

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Due to their lightening effect of freckles and other dark spots on the skin, kojic acid (5-hydroxy-2-(hydroxymethyl)-4-pyrone) and its derivatives have many applications in cosmetics such as a skin-whitening agent via inhibition of tyrosinase, a copper-containing enzyme responsible for melaninsynthesis. Kojic acid can inhibit the formation of dihydroxyphenylalanine from tyrosine in the processof melanin biosynthesis so that it is also used to preserve food color and kill certain bacteria.However, it is known that kojic acid is highly sensitive to sunlight, temperature, and oxygen. Itsdegradation products containing the 4-pyrone may have adverse effect on human health like benzeneto cause serious side effects such as hepatocellular and thyroid adenomas. Therefore, it is required tofind ways in avoiding direct contact with the skin and preventing them from degradation to maximizetheir efficiency. In this work, the layered yttrium hydroxide (LYH) was explored as a host material forthe encapsulation of kojic acid. Resulting kojate-intercalated LYH hybrid showed a potential that theinhibition ability of tyrosinase can be practically maintained without direct contact with the skin.

Poster Presentation : **MAT.P-470**

Material Chemistry

Event Hall THU 11:00~13:00

Selective Gas Sorption and Analysis of Manganese Silicate Hollow Nanospheres

Jin Bae Lee

Research Center for Materials Analysis, Korea Basic Science Institute, Korea

Among the nano-structured materials, the hollow spheres in the dimension from nanometer to micrometer are of significant interest because of property, such as high specific surface, low density, high damping capacity, low thermal conductivity and dielectric permittivity, and can be also used as catalysts, potential drug carriers, fillers, coatings, dyes, artificial cells and photonic crystals.The various hollow nanospheres were prepared by a simple procedure for fabricating hollow nanospheres by hydrothermal method for potential applications as H2 storage materials and CO2 adsorbent. The obtained hollow nanospheres were characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM) and so on.We synthesized various hollow nanospheres as manganese silicate, managnese carbonate, TiO2 and vanadium oxide nanospehres. The hollow nanospheres are approximately uniform in size and the dark/light contrast clearly reveals the hollow nanosphere. In summary, manganese silicate is revealed MnSiO3 having a tetragonal structure in XRD analysis. Mangansese silicate hollow nanospheres have a mean diameter of 7 nm.

Poster Presentation : **MAT.P-471**

Material Chemistry

Event Hall THU 11:00~13:00

Shape controlled synthesis of Cu2O crystals with exposed high-index facets

Young-Duk Huh*, Eung-Dab Kim

Department of Chemistry, Dankook University, Korea

Recently, it has been observed that the catalytic activities of Cu2O microcrystals with exposed high-index facets, such as 26-facets polyhedra and 50-facets polyhedra, are higher than those of Cu2O microcrystals with exposed low-index facets, such as cubes, octahedra, and rhombic dodecahedra. Therefore, the morphology-controlled synthesis of Cu2O microcrystals with exposed high-index facets is important for their potential applications. We demonstrate the facile and rationally-designed synthetic strategy for the Cu2O microcrystals with exposed high-index facets. The morphological evolution of the Cu2O microcrystals from a cube to an octahedron through and a 26-facets polyhedron is examined. A mechanism is proposed to explain the morphological evolution of the Cu2O crystals.

Poster Presentation : **MAT.P-472**

Material Chemistry

Event Hall THU 11:00~13:00

Solid-Solvent Hybrid Additive for the Simultaneous Control of the Macro- and Micro-Morphology in Non-Fullerene-Based Organic Solar Cells

Daehwan Lee, Taiho Park*

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

Most organic solar cells based on a bulk-heterojunction active layer are fabricated with the assistance of high boiling point solvent additives to optimize the phase separation of the donor and acceptor. The macroscopic phase separation can be controlled by this solvent additive. However, the control of the microscopic morphology (e.g., π-π stacking, orientation) of the inside phase is still dependent on the interaction and self-assembly characteristics of each donor and acceptor. In this work, we introduce a solid-solvent hybrid additive on PM6:Y6 solar cells to optimize both the macroscopic phase separation and the microscopic morphology at the same time. For the solvent additive, the well-known 1-CN solvent additive was used. For the solid additive, newly synthesized 3D star-shaped solid additives (Star-A and Star-F), which were delicately designed to achieve adequate electrical properties, electrostatic potential, and geometrical structure, were used to further optimize the microscopic morphology. Grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence wide-angle X-ray scattering (GIWAXS) measurements showed that the star additives not only induce the dense and enhanced microscopic intermolecular π-π stacking within the phase, but also further optimize the phase separation. By adding only 1% star-series solid additives, a significantly enhanced efficiency was achieved from PM6:Y6 solar cells.

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Poster Presentation : **MAT.P-473**
Material Chemistry
Event Hall THU 11:00~13:00

Hollow Structure of $NiFe_2O_4$/rGO Composites as High-Performance Anode Material for Lithium-Ion Batteries

Minseop Lee, Jae-Min Oh[1,*], Seung-Min Paek[2,*]

Chemistry, Kyungpook National University, Korea
[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*
[2]*Department of Chemistry, Kyungpook National University, Korea*

Precursors of $NiFe_2O_4$/rGO composites were prepared through a layer-by-layer (LBL) self-assembly method using only the electrostatic interaction between graphene oxide (GO) and Ni/Fe-LDH. $NiFe_2O_4$/rGO composites with a hollow structure from which the polymer template was removed were successfully obtained after the precursor containing the polystyrene template was heat treated at 470°C in an inert conditions. During the heat treatment process, the Ni/Fe-LDH crystallizes into nickel ferrite ($NiFe_2O_4$) having a spinel structure and is homogeneously distributed among the reduced graphene oxide (rGO) sheets. The distribution of each material was confirmed through HRTEM images and EDX. In addition, the properties of the hollow structure provide a buffer space that can accommodate volume changes even after long-term cycling and enable fast electron and Li ion transport based on the improved accessibility between the electrode and the electrolyte. The electrochemical synergistic effect between rGO sheets and $NiFe_2O_4$ nanoparticles is shown in the rate performance test performed at current densities up to 20000 mA/g and very high discharge capacity of 1423.2 mAh/g achieved at a current density of 100 mA/gIn addition, the structural collapse of the electrode due to the $NiFe_2O_4$ nanoparticles undergoing conversion reaction during the charge/discharge cycle can be alleviated by the rGO sheets, and this result was confirmed through the EIS measurement results measured at various cycles.

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Poster Presentation : **MAT.P-474**

Material Chemistry

Event Hall THU 11:00~13:00

Defective domain control of TiO_2 support in Pt/TiO_2 for room temperature formaldehyde (HCHO) remediation

Youngtak Oh

Center for Environment, Health, Korea

Sustainable and effective formaldehyde (HCHO) remediation at room temperature has significant potential in next-generation indoor environment purification technology. Herein, defective anatase TiO_2 was synthesized using chemical vapor condensation (CVC) and was subsequently impregnated with 0.08 wt% Pt. The resulting Pt/CVC-TiO_2 catalyst was used for the room-temperature conversion of HCHO and exhibited a HCHO removal efficiency of 80% under continuous flow conditions (GHSV 100,000 cm^3 h^{-1} g_{cat}^{-1}) with an initial concentration of 10 ppm with good stability over 600 min. The characterization results confirmed the metallic oxidation state (Pt^0), oxygen vacancies (mainly F centers), disordered domains, and strong interaction between Pt and defective TiO_2 were essential for high activity. Moreover, electron paramagnetic resonance (EPR) analysis showed the consistent stability of the defective domains of CVC-TiO_2, imparting catalytic stability over multiple cycles. This study highlights the synergistic relationship between oxygen vacancies in the TiO_2 support and the resulting HCHO oxidation functionality.

Poster Presentation : **MAT.P-475**

Material Chemistry

Event Hall THU 11:00~13:00

Measurement of Intracellular Viscosity of Living Cells through Fourier Transform Surface Plasmon Resonance (FTSPR)

Sungwoo Lee, Sungho Park[*]

Department of Chemistry, Sungkyunkwan University, Korea

We demonstrate active nanorheology for intracellular viscosity in living cancer cells and fibroblasts using plasmonically active and magnetically responsive nanorods. Electrochemically synthesized Au/Ni/Au nanorods act as “nanotransmitter” which transmits the mechanical motion of nanorods to electromagnetic radiation signal and the received signals are transduced as frequency peaks via Fourier transform surface plasmon resonance (FTSPR) sensing platform which is “signal transducer”. Owing to the combinatorial contribution from magnetic torque and viscous torque exerted onto the Au/Ni/Au nanorods, Au/Ni/Au nanorods exhibit either synchronous or asynchronous mechanical motion. Above a critical threshold of rotating frequency of external rotating magnetic field applied to the Au/Ni/Au nanorods, perturbed dynamics of nanorods led to the disappearance of FTSPR peak, which allows us to measure the local viscosity of medium surrounding nanorods. After a systematic study using bulk viscous glycerol solutions, we applied this method to living cells as a proof of concept and revealed that the intracellular viscosities of cancer cells and normal cells were different. We envision that this active nanorheology with Au/Ni/Au nanorods is an effective and sensitive step towards understanding the physiological properties of cancer cells.

Poster Presentation : **MAT.P-476**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and single particle SERS study of plasmonic all frame-faceted octahedral nanoframes

Jeongwon Kim, Sungho Park[*]

Department of Chemistry, Sungkyunkwan University, Korea

Here, we report the new synthetic method on all frame-faceted octahedral nanoframes by a template-assisted colloidal synthesis. To realize the state-of-the-art complex nanoframes, a stepwise bottom-up process and colloidal chemistry of metals such as reduction, galvanic replacement, etching reaction are designed with Au octahedra nanoparticles as initial templates. By rationally controlling surface chemical reactivity in solution-phase, Pt tripod nanoframes are engraved on the eight faces of the octahedron structures, forming Pt tripod frame-faceted in 3D octahedral nanoframes with high integrity after etching of inner pre-patterned Au. Importantly, AuAg alloy-based plasmonic all frame-faceted nanoframes were successfully achieved after co-reduction of Ag and Au, which generated multiple hot-zones within intra-nanogaps. The highly enhanced electric near-fields within multiple intra-frames enable to achieve a single-particle SERS signal, providing a new platform for the synthesis of complex nanoframe structures. We expect our study can open a new pathway for nano-surface engineering in diverse applications.

Poster Presentation : **MAT.P-477**

Material Chemistry

Event Hall THU 11:00~13:00

Silk fibroin-regulated crystallization of calcium carbonate

<u>Byeongho Park</u>, Sehun Jung[1], Seog Woo Rhee[2,*], Jinkwon Kim[2,*]

Chemistry, Kongju National University, Korea
[1]*department of chemistry, Kongju National University, Korea*
[2]*Department of Chemistry, Kongju National University, Korea*

In this study, we investigated the synthetic processes to regulate the phases and shapes of calcium carbonate formed by the reaction of calcium chloride and sodium carbonate in an aqueous solution containing silk fibroin (SF), sodium dodecyl sulfate (SDS), and poly(sodium-4-styrene sulfonate) (PSS). By varying the ratios of SF, SDS, and PSS, the crystalline calcium carbonate in calcite phase and vaterite phase was selectively synthesized, and the particles were obtained in cube-like, flower-like, and sphere shapes. The thermal decomposition reactions of hybrid composites were investigated by thermal analysis (TGA/DSC), and their ability as flame retardant pigments was tested.

Poster Presentation : **MAT.P-478**

Material Chemistry

Event Hall THU 11:00~13:00

Study on the flame retardant properties of aqueous formulations of clay mineral and natural fibroin

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In this study, we developed the aqueous formulations of eco-friendly flame retardant using clay mineral and natural organic material, and investigated their flame retardant properties. Synthetic hydrotalcite containing hydroxide ions, carbonate ions and water was used as a clay mineral pigment, and fibroin extracted from cocoons was used as a natural organic binder. The thermal decomposition reactions of pigment and binder were investigated by thermal analysis (TGA/DSC). Combustion test (ISO-5660-1) was performed for 10 minutes using a cone calorimeter on a wood specimen coated with the composite film with a uniform thickness. The flame retardant properties were investigated by quantitatively measuring the heat release rate (HRR), oxygen consumption, the amount of released gas (CO_2, CO), and the mass change of the specimen as a function of time.

Poster Presentation : **MAT.P-479**

Material Chemistry

Event Hall THU 11:00~13:00

Oxygen barrier for protecting thermally activated delayed fluorescence dye in organophilic octosilicate

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Thermally activated delayed fluorescence (TADF) dyes have attracted attention in order to increase an electroluminescent quantum efficiency of organic light emitting diode. in order to keep high quantum yield of emission of TADF dyes in air, protection of triplet excited states is important. Moreover, homogeneous molecular environment is also critical issue for quantitative analysis. At these aspects, organically functionalized layered silicate is one of best candidates. In this study, a hybrid of a TADF dye (4CzIPN) and a dioleyldimethylammonium (DODA) intercalated octosilicate was prepared for protection of a triplet excited state of 4CzIPN from oxygen in air.The hybrid was prepared by cation exchange of octosilicate with DODA and intercalation of 4CzIPN by mechanical mixing with an agate mortar and pestle. An external emission quantum yield of the hybrid was 0.71 in air which was higher than that of 4CzIPN powder (0.66). Intensity of TADF of 4CzIPN powder decreased in ambient condition due to oxygen, while that of the hybrid were not different in ambient condition and under N2 atmosphere. The intensity of TADF of the hybrid was larger than that in the 4CzIPN powder in ambient condition and lower than that in the 4CzIPN powder under N2 atmosphere, suggesting that accessibility of oxygen to 4CzIPN was limited in interlayer space of the DODA intercalated octosilicate.

Poster Presentation : **MAT.P-480**

Material Chemistry

Event Hall THU 11:00~13:00

Comparative study on the liquid olefin/paraffine adsorption on ZIF-8

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Linear α α-olefins (LAO) are is an unbranched alkenes, where α α indicates the position of the double bond. Among lLinear α-olefinsAOs, 1-octene isare used as a starting material in wide range of applications, including packaging plastics, high-performing industrial oils, waxes, and surfactants. The separation of LAOs is a major challenge in the petrochemical industry from the catalytic reaction. Specifically, the removal of isomeric paraffin impurities is critically hampered by the minimal boiling point difference in LAOs. Syngas contains many substances with similar boiling points, so it is difficult to separate through simple distillation and consumes a lot of energy. Liquid-phase adsorption has excellent separation efficiency with high selectivity at low temperatures. In this study, ZIF(zeolitic imidazolate framework)-8 Zeolitic Imidazolate Framework (ZIF)has been employed as an adsorbent to separate LAOs from three liquid olefin/paraffin mixtures, 1-octene/n-octane (C8), 1-decene/n-decane (C10), and 1-dodecene/n-dodecane (C12). is a type of metal organic frameworks(MOF). ZIF is a material having a zeolite structure in which organic imidazolate ions are linked around metal ions. ZIF were synthesized by the co-precipitation of Zn2+ using 2-methylimidazole. In this presentation, we have conducted batch-type experiments employing ZIF-8 as an adsorbent to separated α-olefins from three binary liquid-phase olefin/paraffin mixtures, 1-octene/n-octane (C8), 1-decene/n-decane (C10), and 1-dodecene/n-dodecane (C12). The adsorption capacity of both phase olefin and paraffin was analyzed by gas chromatography after the adsorption experiments. The Langmuir and Freundlich isotherms were used to elucidate the interaction between liquid olefin/paraffine and the adsorbent.. assess the adsorption characteristics.

Poster Presentation : **MAT.P-481**
Material Chemistry
Event Hall THU 11:00~13:00

Flow-electrode capacitive deionization cell characterization using electrochemical impedance spectroscopy

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Capacitive deionization (CDI) has been considered as a promising desalination technology because of its high energy efficiency and simple process. When an external voltage is applied to the anode and the cathode, charged salt ions can be separated the electrostatic adsorption onto electric double layer of carbon electrode surface. However, an additional discharging step is required after the charging (desalination) step in order to regenerate the carbon electrode, which limits its desalination performance. Flow-electrode capacitive deionization (FCDI) has been proposed to overcome the disadvantage of a conventional CDI cell because it does not require the discharging process by supplying slurry electrodes, resulting in high salt removal capacity with a continuous desalination operation. FCDI uses the carbon-based slurry electrode and the electrode flows it through the anode and cathode current collector channels. The anode and cathode compartments are separated by cation and anion exchange membranes, and the saline water flows between membranes. In this presentation, the electrochemical performance of FCDI cell as a function of the activated carbon weight percentage in the slurry electrode. The influence of activated carbon amount (1 wt.%, 5 wt.%, 10 wt.%, 15 wt.%, and 20 wt.%) on the electrochemical properties were analyzed using combined electrochemical impedance spectroscopy followed by equivalent circuit fitting and desalination experiments.

Poster Presentation : **MAT.P-482**

Material Chemistry

Event Hall THU 11:00~13:00

Quantitative evaluation method for biofouling inside medical tube

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We developed a quantitative method to evaluate the degree of biofouling regard to the medical tube. Sticky protein, mucin (M), was selected as model foulant and polyvalent basic dye, alcian blue (AB), was utilized as colorimetric indicator. As AB readily binds to M, the pre-mixed AB-M complex was utilized as colorimetric foulant and contacted with medical tube either by impregnation or circulation. After a certain time period, the tube was collected and the loosely bound AB-M foulant inside the medical tube was gently removed by tilting the tubes. Then, the tube with surface bound AB-M was dried. Finally, the tightly bound foulant, AB-M, was chemically detached by 35% H2O2 treatment. The amount of AB-M strongly bound at the surface of tube was quantified by measuring optical density and 595 nm. We applied this method to two kinds of medical tube: one with pure PVC and the other one with TiO2 nanoparticle dispersed in PVC. Based on impregnation test, the PVC tube with and without TiO2 showed 0.066 and 0.198 mg-AB-M/cm2 of fouling effect, respectively, suggesting that the existence of TiO2 nanoparticle was effective in biofouling resistance. Similarly, circulation test also exhibited antifouling effect of TiO2 containing PVC, showing 0.097 mg-AB-M/cm2 of fouling which was 2.57 times lower than that of pure PVC tube, 0.249mg-AB-M/cm2.

Poster Presentation : **MAT.P-483**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation and application of Sr_2YF_7:Yb^{3+}, Er^{3+}, Eu^{3+} for solar cell

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Lanthanide-doped fluorescent upconversion materials, in which low energy photon excitation results in higher energy photon emission, have been attended because they exhibit a lot of advantages such as high penetrated length, and high ratios of signal and noise. The fluorescent upconversion originates from the special electronic property of lanthanide ions. Sr_2YF_7 -a fluoride compound- is a promising host of upconversion materials due to its low phonon energy. In this presentation, the optical properties of Sr_2YF_7 doped with Yb^{3+}, Er^{3+}, and Eu^{3+} ions are shown. The prepared material was used as a component of the working electrode for solar cells. The power converted efficiency of the prepared cell improved up to 21%.

Poster Presentation : **MAT.P-484**

Material Chemistry

Event Hall THU 11:00~13:00

Silver-Cadmium Sulfide Yolk-Shell Heteronanostructures with High Optical Interaction for Plasmon-Enhanced Photocatalysis

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The combination of a semiconductor and a plasmonic metal holds great promise for developing advanced photocatalysts. However, the realization of a heteronanostructure that accommodates both materials in an effective way has been a great challenge. Herein, we report a synthesis of a photocatalyst with a yolk-shell heteronanostructure, which contains a plasmonic Ag yolk inside a CdS shell. The sulfidation of Ag nanospheres followed by a controlled cation exchange reaction successfully generated the Ag-CdS yolk-shell nanostructures. The as-prepared heteronanostructures exhibited a prominent enhancement of photocatalytic activity toward hydrogen evolution reaction under visible-light irradiation compared to CdS hollow nanoparticles without the Ag yolk. This improvement can be attributed to the plasmon energy transfer from the Ag yolk to the CdS shell and the yolk-shell structure that enables the multiple reflections of the incident light.

Poster Presentation : **MAT.P-485**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of highly porous carbon materials for advanced adsorbents

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Porous carbon materials have shown great potential in the energy and environmental fields. In particular, they are applied as adsorbents, catalyst supports and electrodes due to their thermal stability, high electric conductivity, high surface area and porosity. Pores can be classified into three groups depending on their pore sizes such as macropores, mesopores, and micropores. Macropores allow rapid mass transport and mesopores have abundant reaction sites for guest molecules. Micropores provide a large surface area for small molecules together with strong adsorption ability. The combination of interconnected pores can greatly enhance their properties and gas adsorption capacity. Recently, a number of strategies have been reported to prepare porous carbons with huge surface area and well-developed porous structure. In this work, porous carbon materials with these intriguing structural characteristics were synthesized including activation procedures to improve the gas adsorption performance.

Poster Presentation : **MAT.P-486**
Material Chemistry
Event Hall THU 11:00~13:00

Characterization and Application of Ordered Mesoporous Carbon with Physical Block and Catalytic Effects

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Nowadays portable electronic devices are used widely and electric vehicle market is growing. It makes secondary batteries important for future innovation. Li-ion battery which is most commonly used has problems with high price and possibility of explosion and also it reaches the limitations of energy density. So Li-S battery is becoming a one of the promising alternatives. It has high theoretical energy density and low cost. Also it is eco-friendly and safe. However, there is the primary problem to be commercialized. That one is called shuttle effect, which means dissolution of polysulfides into the electrolyte in the repetitive charging and discharging. It makes capacity decrease and internal resistance increase. To minimize the shuttle effect, we modified ordered mesoporous carbon(OMC) materials. Carbon materials which have good conductivity are used with sulfur because the sulfur is non-conductive. Especially the OMC has thermal and chemical stability, high surface area and high pore volume. First, we synthesized the OMC materials with micropores by introducing silica nanoparticles as physical block. We expected that polysulfides with long chain could be blocked because of the small pore size. Also we loaded platinum nanoparticles on the OMC for catalytic effects. Platinum nanoparticles could catalyze the reaction of polysulfides so shuttle effect could be alleviated.

Poster Presentation : **MAT.P-487**

Material Chemistry

Event Hall THU 11:00~13:00

One-Pot Synthesis of Pd-Pt-Ag Ternary Alloy Hollow Nanostructures with Controlled Morphologies for Ethanol Electrooxidation

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Rational design and synthesis of multimetallic hollow nanostructures (HNSs) have been of great attention due to their structural and compositional advantages for the application in electrocatalysis. Herein, the one-pot synthesis of Pd-Pt-Ag ternary alloy HNSs with controllable morphologies through a self-templating approach without any pre-synthesized templates is reported. Simultaneous reduction of multiple metal precursors by ascorbic acid in the presence of cetyltrimethylammonium chloride (CTAC) yielded initially metastable Pd-Ag nanocrystals, which can act as a self-template, and subsequent galvanic replacement and reduction led to the formation of the final Pd-Pt-Ag HNSs. The size and hollowness (the ratio of inner cavity diameter to outer diameter) of the HNSs could be tuned through control over the concentration of CTAC. This can be attributed to the manipulated reduction kinetics of multiple metal precursors with the change in the CTAC concentration. The prepared Pd-Pt-Ag HNSs exhibited improved catalytic performance for ethanol electrooxidation due to their large active surface areas and ternary alloy composition.

Poster Presentation : **MAT.P-488**

Material Chemistry

Event Hall THU 11:00~13:00

Palladium-Coated Gold Nanoparticle Trimers for Efficient Light Exploitation

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Incorporation of catalytically active materials into plasmonic metal nanostructures can efficiently merge the reactivity and energy-harvesting abilities of both types of materials for visible light photocatalysis. Herein, we explore the influence of electromagnetic hotspots in the ability of plasmonic core−shell colloidal structures to induce chemical transformations. For this study, we developed a synthetic strategy for the fabrication of Au nanoparticle (NP) trimers in aqueous solution through fine controlled galvanic replacement between Ag nanoprisms and Au precursors. Core−shell Au@M NP trimers with catalytically active metals (M = Pd, Pt) were subsequently synthesized using Au NP trimers as templates. Our experimental and computational results highlight the synergy of geometry and composition in plasmonic catalysts for plasmon-driven chemical reactions.

Poster Presentation : **MAT.P-489**

Material Chemistry

Event Hall THU 11:00~13:00

Fabrication of a SERS substrate using silver nanoparticles on etched silica particles

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In this work, we report the preparation of a SERS substrate using non-close packed monolayer array of silica nano-spheres (NPMASNs) as a template decorated by uniform silver nanoparticles (AgNPs) synthesized by droplet microfluidics, which includes techniques of dip-coating of silica nano-spheres (SNs), aqueous hydrofluoric etching and self-assembly monolayer (SAM) of AgNPs. Utilizing this method, a SERS substrate based on well-ordered nano-particles of silica@AgNPs monolayer array can achieve. High voltage field effect scanning electron microscopy (FESEM) and ultra-violet-visible (UV–VIS) spectrophotometry techniques performed to investigate the surface morphology and optical properties of the as fabricated substrate. To investigate the Raman enhancement of the SERS substrate, Thiabendazole (TBZ) was selected as analyzed target molecules, which exhibit good homogeneity, reproducibility and stability with limit of detection (LOD) as low as 10^{-9} mol/L.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-490**

Material Chemistry

Event Hall THU 11:00~13:00

Mesoporous WO_3/SBA-15 catalyst for conversion of glycerol into 1,3-dioxolane-4-methanol

<u>Jin Seo Park</u>, Zhengyang Li[1], Ji Man Kim*

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Biodiesel has gained a considerable attention in recent years. The production of biodiesel involves a transesterification of vegetable oils to afford biodiesel and glycerol. Glycerol can be transformed into diverse derivatives. Among them, acetalization of glycerol has been reported to yield five and six membered acetals. In this research, glycerol conversion with acetone has been studied using mesoporous WO_3/SBA-15 as a catalyst. A series of catalysts with varying WO_3 loadings (5~20 wt%) were prepared by incipient wetness impregnation method. The catalysts were characterized with XRD, Raman spectroscopy, SEM, N_2 sorption analysis, and NH_3-TPD. In the catalytic experiment, 10 wt% WO_3/SBA-15 was found to be the most active catalyst. The catalyst exhibited 97% conversion with 97% selectivity for 1,3-dioxolane. Although the catalytic performance decreased in the 5th catalytic run, the catalyst was regenerated by calcination in 6th catalytic run. The excellent performance of the catalyst is mainly due to their high specific surface area and strong surface acid property.

Poster Presentation : **MAT.P-491**

Material Chemistry

Event Hall THU 11:00~13:00

Using CeO_2 as supporting materials for multi-branched PtNi nanocrystals and investigation of their bifunctional electrocatalytic performances

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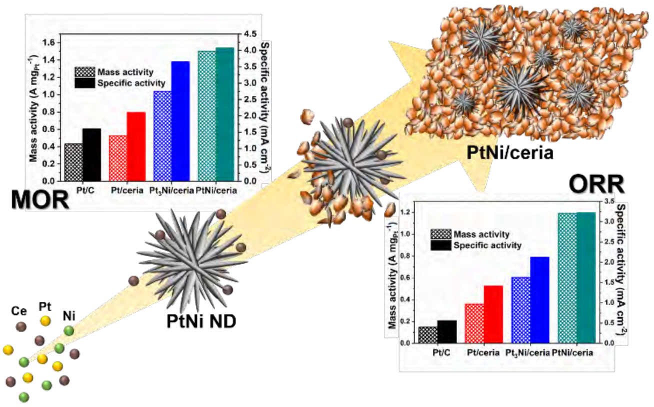
Devising efficient routes to realize hybrid materials consisting of intimately coupled metal nanocatalysts and nonstoichiometric metal oxides with finely controlled configurations is highly desirable to develop advanced fuel cell catalysts. Here, we report a facile one-pot synthesis strategy for the formation of closely coupled metal (PtNi alloy)-metal oxide (CeOx, ceria) hybrid nanostructures. Heating an oleylamine/oleic acid solution of mixed metal (Pt, Ni, and Ce) precursors yielded well-defined PtNi/ceria hybrids, in which PtNi alloy nanodendrites with multiple branches are well dispersed on small-grained ceria nanosheets. Due to their small grain size, the ceria nanosheets in the hybrids contain abundant oxygen vacancies and have high conductivity. The prepared PtNi/ceria hybrids exhibited outstanding electrocatalytic activity and stability toward both methanol oxidation and oxygen reduction reactions in comparison to their carbon-supported counterparts and a commercial catalyst, which can be attributed to the synergistic effects of Ni component and ceria on the enhancement of electrocatalytic function. The current strategy will find use in the design of optimal multicomponent catalysts for intended reactions.



Poster Presentation : **MAT.P-492**

Material Chemistry

Event Hall THU 11:00~13:00

Poisoning of Ag-M Bimetallic Nanocatalysts by Silver Halides and Their Chemical Regeneration

Han-Jung Ryu, Jae-Seung Lee*

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Poisoning of heterogeneous catalysts is an important issue, because it can significantly deteriorate catalytic properties. Despite their importance, however, the poisoning of Ag-M bimetallic nanoparticle (biNP) catalysts has not been investigated with regard to the effect of silver halide (AgX) byproducts which are often unintentionally produced during the synthesis by the ligands of metallic precursors. To address this issue, we synthesized Ag-Pd and Ag-Pt biNP catalysts with controlled shapes and compositions, and investigated the partial deactivation of their catalytic properties by the chlorometallate precursor-induced formation of AgCl. Importantly, we discovered chemical regeneration method for enhancing the catalytic properties of the biNPs using ascorbic acid, which removed AgCl by reduction into Ag. Moreover, the structures of the biNPs were maintained after AgCl removal using ascorbic acid, which is a significant advantage over AgCl removal using conventionally used NH_3. This study is the first to report chlorometallate precursor-induced biNP catalyst poisoning and its chemical regeneration. Our investigation can be used as a guideline for the controlled synthesis of biNPs of high purity and their efficient applications in heterogeneous catalysis.

Poster Presentation : **MAT.P-493**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of Highly Stable Ag-Te nanoparticles through Galvanic Replacement and Their Application to Breast Cancer Photo-Therapy

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Silver-containing nanoparticles have been widely applied to the biosensing and biomedical fields based on their unique physicochemical properties, including prominent anti-cancer/bacterial effects and plasmonic characteristics. However, the disadvantage of being vulnerable to oxidation is considered a typical limitation, and overcoming it is a given mission. Here, to secure the stability of the particles, elliptical nanoparticles with a mixed composition of Ag and Te (AgTeNPs) were made through a galvanic replacement reaction between Ag(I) precursor and rod-shaped Te nanotemplates (TeNRs). We also confirmed highly efficient photothermal conversion under the near-infrared laser irradiation based on the incredible absorption cross-section of AgTeNPs. In combination with colloidal stability and low cytotoxicity of AgTeNPs, selective photothermal therapy was achieved on two types of breast cancer cells. The discovery of Ag-based nanomaterials with such anticancer effects is expected to be a new candidate with therapeutic potential.

Poster Presentation : **MAT.P-494**

Material Chemistry

Event Hall THU 11:00~13:00

Precursor Heterogeneity Combined Morphology Control of Mo-Te Nanostructures for Cancer Photo-Theranostics

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The controlling size and morphology of nanoparticles are crucial whether such nanoparticles can be applied to a specific research field such as cancer therapy. Here, we introduced the synthesis of nanostructures with the composition of Mo and Te from heterogeneous precursors, including solution dispersed solid polyoxomolybdates (POMs) and dissolved tellurite anions. as the concentration of POMs increased, smaller and shorter elliptical nanostructures were evolved. According to the size dimension decrease, we denoted obtained nanostructures as nanoleaves, nanospindles, and nanorices. After confirming cell viability under the treatment of each nanostructure, we applied nanorices in cancer theranostics based on their excellent biocompatibility and the photothermal conversion efficiency. Mo-Te nanorices exhibited excellent photothermal and photodynamic therapeutic efficacy as well as photoacoustic signals. By demonstrating the concurrence of photoconverting properties through heat and ultrasonic waves from the nanoparticles, we broaden the possibility to apply appropriate nanoparticles to cancer therapy and imaging at the same time from nanoparticles with Mo-Te composition.

Poster Presentation : **MAT.P-495**
Material Chemistry
Event Hall THU 11:00~13:00

Solvent-Controlled Galvanic Replacement to Synthesize Mushroom-Like Gold Nanoplates for Cancer Phototherapy

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Tailored nanoparticles exhibit unique physicochemical properties based on their size, internal-and external-structures, and elemental compositions. In this study, mushroom-like gold nanoplates (mAuNPs) were successfully synthesized via solvent-controlled galvanic replacement reaction between formerly reported silver nanoplates and Au(III) precursors. By fostering the co-solvent environment and controlling the volumetric concentration of each reaction solution mixed with deionized water and ethylene glycol, the morphologies of mAuNPs were varied from porous nanoplates to nanoring decoration or tail growth. After thorough characterizations, the mAuNPs constructed as porous gold nanoplate head and a hollow nanotube tail were applied to photo-triggered biomedical application. The mAuNPs showed excellent photothermal conversion efficiency under the irradiation of near-infrared laser. Based on the superior biocompatibility of mAuNPs, , we finally achieved the photothermal cancer therapeutic application. Taken together the result, we expected that the present mAuNPs could be a new candidate for noble metal nano-photo-carrier for cancer therapy fields.

Poster Presentation : **MAT.P-496**

Material Chemistry

Event Hall THU 11:00~13:00

Morphology Dependence of Mesoporous Carbon and its Application on Lithium-Ion Battery

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Morphology is relatively simple but a powerful characteristic of all kinds of materials. Especially when it is used as active material in lithium-ion batteries, it affects the pathway of lithium-ion during charge/discharge process. Also, it affects the contact area of active materials which eventually has an effect in conductivity. In this article rod-type, spherical type mesoporous carbon was synthesized using nano-replication method. Rod/spherical type SBA-15 was used as silica template. In order to give morphology difference, CTAB was used as an additive during synthetic process.After synthesizing these materials, they were characterized using X-ray diffraction, nitrogen adsorption isotherm analysis, and electron microscopy. Cell performance was confirmed using JEIO TECH code NO. AAH220412K.

Poster Presentation : **MAT.P-497**

Material Chemistry

Event Hall THU 11:00~13:00

Amplified Spontaneous Emission in colloidal Quantum dot under nanosecond optical pumping

Suhyeon Kim, Hye Kyeong Kwon, Jiwon Bang*

Chemistry, Wonkwang University, Korea

Colloidal quantum dots (QDs) have obtained significant attention for versatile gain material due to their solution processability and size-tunable optical transitions. The requirement for light amplification of QDs is population inversion, and therefore, biexciton is necessary for the band-edge state. However, the existence of strong Coulomb interactions in the three-dimensional quantum confinement colloidal QDs used as gain media have been hindered by greatly increasing the rate of multi-exciton Auger decay. To use practical implementation of CQD lasers, operation with nanosecond or longer pulse duration is required but laser demonstrations of QDs have been mostly used ultrafast (sub-ps) optical pulse excitation to preserve population inversion state. Herein, we demonstrated amplified spontaneous emission (ASE), a precondition for the lasing action, of the colloidal CdSe/CdS/ZnS QDs under nanosecond optical pumping. When the QDs in a close-packed structure is optically pumped by a frequency tripled Nd: YAG laser emitting 4 ns pulses with a 355 nm, emission from the QD film edge is abrupt increase with increasing pump power in output intensity and reducing the emission linewidth on the higher-energy side of the photoluminescence band. This result represents a clear transition from photoluminescence to ASE. The blue shifting ASE peak of the QDs indicated repulsive charge carriers interaction in biexciton state, which implies that our QDs represent the quasi-type II band structures. The spatially separated carrier distribution in quasi-type-II CdSe/CdS/ZnS QDs expected to reduce the unwanted Auger process and promote the radiative recombination of biexciton.

Poster Presentation : **MAT.P-498**

Material Chemistry

Event Hall THU 11:00~13:00

Stabilized oil-in-water emulsion containing deoxycholic acid utilizing 2-dimensional layered double hydroxide

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Deoxycholic acid (DA), as a metabolic byproduct in living system, is known to dissolve subcutaneous fat easily. Although the injection of DA solution has been widely applied, transdermal application of DA has been limited due to the molecular aggregation of DA at slightly acidic emulsion. In this research, layered double hydroxide (LDH) with 2-dimensional nanosheets, was utilized to suppress molecular aggregation and to finally increase the stability of the oil-in-water emulsion with DA moiety. For effective molecular arrangement, solubilized DA was coprecipitated with Mg2+ and Al3+ to produce DA intercalated LDH (DA-LDH). Then either DA or DA-LDH was added to emulsion consisting of medium-chain triglyceride. According to dynamic light scattering, it was confirmed that the formulation of DA-LDH maintained hundreds of nanometer sizes upon dilution, while the formulation having naked DA readily aggregated to large micelles upon dilution. It may be attributed to the molecular aggregation of DA along with dilution. Furthermore, the time-dependent colloidal behavior of both emulsion was monitored by Turbiscan(R). While the naked DA containing emulsion showed 9% of transmittance change during 24 h, the DA-LDH containing formulation resulted in 4% of transmittance change. Although both formulation showed global agglomeration during 24 h, the degree of agglomeration was lower in DA-LDH formulation than DA formulation, showing 4% and 9% of transmittance change, respectively.

Poster Presentation : **MAT.P-499**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation of InP quantum dot linked TiO2 nanoparticle composites with enhanced visible light induced photocatalytic activity

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Environment friendly InP based quantum dots (QDs) are expected to be ideal visible light harvesting materials thanks to their unique photophysical properties. Here, we report a combination of visible light response InP/ZnSe (core/shell) QDs with TiO2 nanoparticles (NPs) as a visible light photocatalysts. Strong negative charged sulfonate functional ligands were introduced on the InP/ZnSe QD surface, and the negative charged InP/ZnSe QDs were electrostatically conjugated to the oppositely charged TiO2 NP surface. The scanning electron microscopy images confirmed that QDs are densely coated with whole TiO2 surface, and the QD-TiO2 interaction is maintained in acidic and neutral medium. The band edge photoluminescence (PL) intensity was reduced with remarkably shortening the average PL lifetime of the QD after being linked to TiO2 indicating that the photoexcited electrons in InP/ZnSe QDs were efficiently transferred to the TiO2. The spatially separated photoinduced charge carrier with suppressing charge recombination of the InP/ZnSe QD-TIO2 enhanced the photocatalytic rhodamine B dye degradation efficiency. Both charge generation over a broad solar spectral range and electrons-holes separation capabilities of the InP/ZnSe QD-TIO2 can provide many new possibilities for solar energy harvesting systems.

Poster Presentation : **MAT.P-500**

Material Chemistry

Event Hall THU 11:00~13:00

Thermodynamic and kinetic comprehension of methylene blue adsorption on the porous silicate synthesized from industrial waste

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Department of Energy and Materials Engineering, Dongguk University, Korea

Highly porous silicate materials were prepared by treating industrial waste slag with appropriate acid solution. Slag which consisted of metal oxides of Si, Mg, Ca, Fe, Mn, and etc. was ground and fine particles were separated with 400 mesh (37 microns) sieves. Then, 3 mol/L and 6 mol/L of hydrochloric acid were added to each powder to dissolve metal species and to remain silicate moiety. The powder sample were designated as S1 (HCl 3 mol/L) and S2 (HCl 6 mol/L). The nitrogen adsorption-desorption isotherms and the X-ray photoelectron spectroscopy showed that the higher concentration of acid produced the more dissolving of metal species resulting in increasing specific surface area pore volume. The pore size distribution analyses showed that the mesopore and micropore were developed, respectively, for S1 and S2. We confirmed that inter-particle space of silicate particles in both samples established porous network, by the transmission electron microscopic images. The adsorption performance of both samples was investigated in aqueous condition utilizing methylene blue as target adsorbate. Adsorption kinetics of S1 and S2 under 25 degrees and 50 degrees showed pseudo-second-order kinetics with higher kinetic constant for S1. The mesoporous silicate adsorption of methylene blue solution was more effective than the microporous silicate. The adsorption isotherms revealed that the adsorption of both samples followed Freundlich model with higher constant for S1. Both kinetic and thermodynamic results strongly indicated that the silicate adsorption was facilitated in S1 with mesoporous structure compared with S2 with micropores.

Poster Presentation : **MAT.P-501**

Material Chemistry

Event Hall THU 11:00~13:00

Indium Phosphide Magic Sized Clusters: Doping and Chirality Control

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Chiral materials are in great interest due to their remarkable application possibilities in fields such as asymmetric catalysis, negative refractive index materials, polarization control, and even in gene engineering. While recent chiral nanomaterial researches are generally focused on II-VI group, nearly none of the chiroptical properties of III-V group nanomaterials nor quantum dot growth intermediates were reported. Herein, we have aimed on understanding the chiroptical activities of III-V group quantum dots growth intermediates, also known as the magic sized clusters (MSCs). We introduce chiral InP MSCs with unprecedented large circular dichroism signals compared to previously reported chiral semiconductor nanocrystals. To investigate the chiroptical origins of our chiral MSCs, characterizations using XPS, FT-IR, Raman, XRD, TGA, and EXAFS were conducted to explore ligand geometry and structural properties. We discovered that our chiral MSCs consists two types of chiral ligand configurations: single anchoring with thiolate group, and double anchoring with both thiolate and carboxylate group. By structural characterizations, the inorganic core is observed to exhibit polytwistane-like structures. Similar sized chiral InP QD was prepared, whereas its optical activity was nearly unobservable. We speculate that low crystal symmetry and large transition dipole moments may be the clue to the high chiroptical activity of MSCs. Using chiral InP MSCs as templates, we could synthesize InP QD, maintaining substantial chiroptical activity. Also, we introduced halide atoms (Cl, Br, I) as dopants into MSCs, which was also CD-active. Our findings emphasize the unique characteristics of MSCs as prospective chiral materials and gives intuition on designing chiroptical nanomaterials.

Poster Presentation : **MAT.P-502**
Material Chemistry
Event Hall THU 11:00~13:00

Synthesis strategy of carbon nitrides 2D Materials Using Covalent Modification and Their Electroluminescence Performance

Jinyoung Son, Seokhyeon Jeon[1,*], Sangjoon Park[1,*], Sungjin Park[1,*]

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Carbon nitrides (C3N4) show excellent properties in various optical and optoelectronic applications. However, their application to electoluminescenece (EL) devices is impeded by the scarcity of production methods of homogeneous dispersion in organic solvents, which are absolutely required for device production. Herein, a strategy to betide stable dispersion of fluorescent, 2D C3N4 materials, and light-emitting diodes (LEDs) based on them is designed. Urea-driven C3N4 (UCN) was dispersed effectively in organic solvents by methoxy-benzene diazonium salt treatment. Experimental and theoretical studies show that MD treatment passivates the surface defects of the UCN. The final LED devices display bright green luminescence with an external quantum efficiency of 0.91 %. This accomplished result opens an era of C3N4 emitters as future promising light emitters in displays and solid-state lighting.

Poster Presentation : **MAT.P-503**

Material Chemistry

Event Hall THU 11:00~13:00

Quantum Dot Composite Colloids with Layer-by-Layer Shell and Their Biological Self-assemblies for Signal Amplified Detection

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The quantum dot composite colloid (QDCC) can be defined as a colloid that contains multiple QDs and endows colloidal properties using proper matrices such as pre-formed polymer beads, silica template, lipid, and polymersome. Herein, we report polyelectrolyte shell decorated QDCCs, which were decorated by cationic (polyethylenimine, PEI)/anionic (poly(sodium 4-styrene sulfonate), PSS) polyelectrolytes in a Layer-by-Layer (LbL) fashion over cores of amphiphilic PEI-derivative composites (QD-amPEI). Sophisticatedly controls over the structural plasticity and colloidal stability could be obtained by tuning the LbL shells of QDCCs that include QDCC shell permeations of ions, fusion/fission of QDCCs that accompany partial exchange between the payloads, and enhanced colloidal stabilities in a broad pH range and high salt concentrations. The outer layer of QDCC shells was tethered by amines, carboxylates, zwitterionic moieties, or a combination of those, which endowed the QDCCs with flexible bioconjugation capability and a very low non-specific adsorption level. As a proof-of-concept experiment, a signal amplification was demonstrated using biotin-avidin motif-assisted biological self-assembly of QDCCs that are either biotin or avidin tethered. Using c-reactive protein (CRP) as a target biomolecule, the signal amplification was applied to an FL immunoassay platform, where rapid (~ 6 minutes) and sub-picomolar sensitive detection was successfully achieved.

Poster Presentation : **MAT.P-504**

Material Chemistry

Event Hall THU 11:00~13:00

Detection of tau protein by using bioactivated carbon nanotube network on microfilter paper sensor Alzheimer's disease diagnosis.

Jiyeong Park, Jihyeon Mun[1], Songmi Bae[2], Don Kim[2,*]

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[2]*Department of Chemistry, Pukyong National University, Korea*

One of the biomarkers to diagnosis Alzheimer's diseases (AD) is tau proteins (TPs). TPs are originated from the aggregation of beta amyloid in the brain and causes dementia. By this time, the detection of TP requires sensitive and expensive sophisticated instruments and are not applicable at the point-of-care (POC). We present an easy, fast, and inexpensive method to assay TP with the TP targeting synthetic-DNA (aptamer) modified carbon nanotubes (TPTA-CNTs). TP immunosensor sensor was prepared by the even deposition of TPTA-CNTs on filter paper. The electrical resistance change of the senor was measured to analysis the level of TPs. In the preliminary detection experiment, the TP sensor could assay in the range of 0 – 80 ng/mL TP, with analytical sensitivity of 0.00122 (ng/ml)$^{-1}$ and limit of detection of 4.8 ng/mL, within 90 min. This economical method should be improved for the real application, but the method can detect much faster than the most common detection method, enzyme-linked immunosorbent assay (ELISA, 6 h).

Poster Presentation : **MAT.P-505**

Material Chemistry

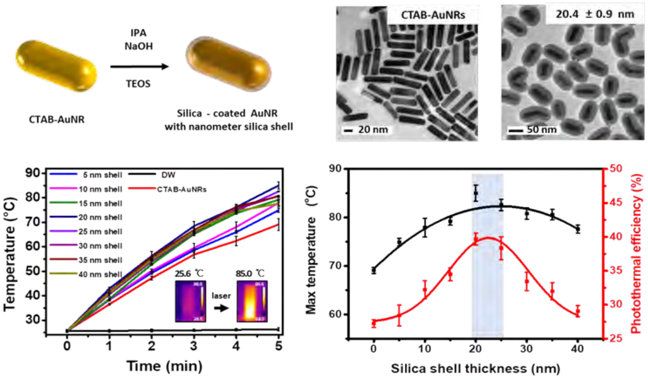
Event Hall THU 11:00~13:00

Precise control over the silica shell thickness and finding the optimal thickness for the peak heat diffusion property of AuNR@SiO_2

Wonseok Yang, Dongkwon Lim*

KU-KIST Graduate School of Science and Technology, Korea University, Korea

Silica-coated gold nanorods (AuNRs) exhibit significantly enhanced photothermal effects and photoacoustic (PA) signal intensities, which is beneficial for various nanophotonic applications in materials science. However, the silica shell thickness for optimum enhancement is not fully understood and is even controversial depending on the physical state of the silica shell. This is because of the lack of systematic investigations of the nanoscale silica shell thickness and the photothermal effect. This study provides a robust synthetic method to control the silica shell thickness at the nanoscale and the physical state-dependent heat diffusion property. The selected base and solvent system enabled the production of silica-coated AuNRs (AuNR@SiO_2) with silica shell thicknesses of 5, 10, 15, 20, 25, 30, 35, and 40 nm. AuNRs with a 20 nm silica shell showed the highest photothermal effect with a 1.45-times higher photothermal efficiency than that of AuNRs without a silica shell. The low density of the silica shell on the AuNRs showed a low photothermal effect and photostability. It was found that the disruption of cetyltrimethyl ammonium bromide (CTAB) layers on the AuNRs was responsible for the low photostability of the AuNRs. The simulation study for the heat diffusion property showed facilitated heat diffusion in the presence of a 20 nm silica shell. In a cell-based study, AuNRs with a 20 nm silica shell showed the most sensitive photothermal effect for cell death. The results of this robust study can provide conclusive conditions for the optimal silica shell thickness to obtain the highest photothermal effect, which will be useful for the future design of nanomaterials in various fields of application.


CTAB-AuNR
IPA
NaOH
TEOS
Silica - coated AuNR
with nanometer silica shell
CTAB-AuNRs
20 nm
20.4 ± 0.9 nm
50 nm
Temperature (°C)
Time (min)
5 nm shell
10 nm shell
15 nm shell
20 nm shell
25 nm shell
30 nm shell
35 nm shell
40 nm shell
DW
CTAB-AuNRs
25.6 ℃
laser
85.0 ℃
Max temperature (°C)
Photothermal efficiency (%)
Silica shell thickness (nm)

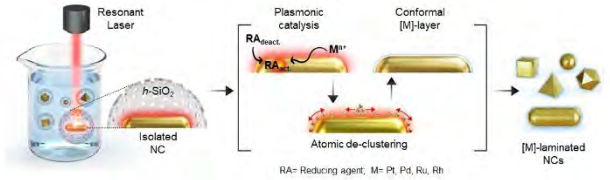
Poster Presentation : **MAT.P-506**
Material Chemistry
Event Hall THU 11:00~13:00

Light Induced Atomically Thin Metal Laminations on Plasmonic Nanocrystals for Efficient Catalysis in Living Cells

Anubhab Acharya, Trimbak Mete, In Su Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Developing new strategies conveying impressive photocatalytic functionalities in plasmonic nanocrystals (NCs) are in demand due to its huge potential in wide range of applications, such as catalysis, electronics, and displays. Despite having an enormous prospect of plasmonic hybrid integrated with catalytic metals, the methods for conformal deposition of catalytic noble metals on plasmonic NCs to a critical limit of few atomic-layer are scarce. Our work introduces “confine and shine” strategy to uniformly cover the distinct surface curvatures of plasmonic NCs with conformal ultrathin layers of various catalytic metals, similar to the process of lamination. Instead of following any kinetic anisotropic metal deposition pathway, the confined environment of hollow silica employs a platform to deposit catalytic metals in an epitaxial skin-like manner with self-limited deposition ability under near-infrared laser. The metal laminations preserve the hallmark plasmonic property of the core part by eliminating any non-radiative damping that usually caused by thicker metal shell. Consequently, the plasmonic-catalytic hybrid can perform diverse photocatalytic chemical transformations with high efficiency and remarkable stability.



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Poster Presentation : **MAT.P-507**

Material Chemistry

Event Hall THU 11:00~13:00

Antioxidant Nanogels loaded with Cesium Lead Bromide Perovskite for Sensing Roxithromycin in Animal-derived Food Products

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Department of Chemistry, Changwon National University, Korea

Luminescent inorganic lead halide perovskite nanoparticles are poorly stable in aqueous conditions, limiting their use as optical sensors. In this study, novel $CsPbBr_3$-loaded MIP nanogels with improved water stability were developed. Multifunctional MIP nanogels with antioxidant function and hydrophobic cavities were synthesized from HEMA derivatives in the presence of roxithromycin as a template. $CsPbBr_3$ nanoparticles with a size distribution of 197 ± 71 nm were loaded into pre-synthesized MIP nanogels by in-situ synthesis. The discovered $CsPbBr_3$-nanogel has high stability to oxygen/moisture and improved stability to an aqueous solvent. The developed $CsPbBr_3$-loaded MIP nanogels demonstrated selective and sensitive roxithromycin detection, with a limit of detection determined to be 1.7 10 5 g/mL. (20.6 pM). Moreover, the practical application for the quantitative determination of roxithromycin in animal-derived food products showed an excellent analytical performance with good recovery results. The achieved stability of $CsPbBr_3$-loaded MIP nanogels makes them an ideal candidate for application as a sensor.

Poster Presentation : **MAT.P-508**

Material Chemistry

Event Hall THU 11:00~13:00

Solvent Additives Coordination Effect on PbI_2 Precursor and High-Performance Perovskite Solar Cells

Hyungwoo Kim, Kwanyong Seo*

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

Organic-inorganic hybrid perovskite solar cells, which can be fabricated via a solution process technology, have attracted much attention regarding high efficiency and low fabrication cost. In particular, the formation of high-quality pin-hole-free perovskite layers with large grains would be a key to the high power conversion efficiency (PCE) of solar cells. Here, we report the effect of solvent additives on perovskite formation regarding Gutmann donor number (D_N) in PbI_2 precursor solution through the two-step spin-coating process. Among the various solvent additives, dimethyl sulfide (DMS) has a high D_N of 23.5 $kcal \cdot mol^{-1}$. The PbI_2 precursor solution with DMS leads to the formation of perovskite thin film with a large grain and excellent electrical properties. The power conversion efficiency of our mixture of perovskite layers $(FA_{0.7}MA_{0.3})Pb(I_{0.7}Br_{0.1}Cl_{0.2})_3$ based solar cell achieves a maximum PCE of 21.2% under AM 1.5G illumination. Our work suggests enormous potential for significant performance improvement of perovskite solar cells via solvent engineering.

Poster Presentation : **MAT.P-509**

Material Chemistry

Event Hall THU 11:00~13:00

The synergy between H_2O adsorption-accelerating $CuCrS_2$ and active Co_9S_8 phase to facilitate hydrogen evolution in neutral media

Ye Ji Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Generating hydrogen, an eco-friendly energy carrier, through electrochemical water splitting from the neutral media has attracted considerable attention due to the much less corrosion of the water electrolyzer and the feasibility of the direct usage of seawater sources without pH adjustment. To enhance the catalytic performance in neutral media by modulating the HER mechanism, electrocatalysts with dual-site were required for facilitating fast water adsorption/dissociation and sequential hydrogen desorption, respectively. Therefore, designing the well-defined heterostructures by integrating the H_2O adsorption-active materials with HER-active materials is a promising strategy to heighten the HER performance. Herein, we synthesized a well-defined hetero-nanostructure with extended grain boundaries by interfacing the metal sulfides with an oxophilic matrix. The efficient charge redistribution at the interface is significantly enhanced the catalytic performance. This study provides a promising design strategy to synthesize the electrocatalysts with hetero-interface and a realization to understand the fundamental HER mechanism in neutral media.

Poster Presentation : **MAT.P-510**

Material Chemistry

Event Hall THU 11:00~13:00

Metal-Chelated Polymeric Hybrid Nanostructures for Luminescence Resonance Energy Transfer

Sang-Min Lee

Department of Chemistry, The Catholic University of Korea, Korea

We present a facile one-pot strategy to achieve a metal-chelated nanoscale platform that enables a highly efficient luminescence resonance energy transfer (LRET) process for the monitoring of organic cargo release. To this end, Eu(III) as a lanthanide luminophore was employed to induce the metal-mediated self-assembly of chelating block-copolymers in the presence of fluorescent nile blue (NB) as an organic cargo, which can then form the nanoscale assemblies containing a hybrid polyionic complex of Eu(III) and NB for LRET pairs. Exploiting this nanoplatform that allows for the intermolecular distance-sensitive LRET process, we further demonstrate that the facile monitoring of NB release from the carriers was made possible upon the addition of serum albumin as a protein reservoir for the released guest molecules.

Poster Presentation : **MAT.P-511**

Material Chemistry

Event Hall THU 11:00~13:00

Light-Responsive Nanofibers Containing Gold Nanorods for On-Demand Drug Delivery Systems

Junkee Kim, Myoung-Hwan Park[1,*]

Department of Convergence Science, Sahmyook University, Korea
[1]*Department of Chemistry, Sahmyook University, Korea*

On-demand drug delivery systems using stimuli-responsive nanofibers are receiving a lot of interest. Near-infrared (NIR)-responsive nanofibers can provide a platform for cancer therapeutic drug release profiles to be established by on-demand delivery of specific amounts of therapeutic agents. Nanomaterials such as gold nanorods (GNRs) having NIR absorbance generate heat in response to NIR irradiation through a plasmon resonance effect. In this study, we developed Poly(N-isopropylacrylamide) (PNIPAM) composite nanofibers containing GNRs. PNIPAM is thermal-responsive polymer, and nanofibers have the ability to expand and contract. Electrospun nanofibers can efficiently transport large amounts of therapeutic agents because of their high surface area to volume ratio. This platform can be used to introduce and control hydrophilic and hydrophobic drugs. Stimuli-responsive nanofibers composed of GNRs and PNIPAM were used to create a controlled drug delivery system. The heat generated by GNRs due to NIR irradiation causes the nanofibers to contract due to the thermal response of PNIPAM to control drug release. Cellular investigations confirmed the capability of light-responsive nanofibers as on-demand drug delivery platform, highlighting the advantages of the swelling and deswelling properties of nanofibers and on-off drug release behavior with excellent bio compatibility. Additionally, this platform has the potential to improve the efficacy of complex cancer treatments by combining multiple drugs.

Poster Presentation : **MAT.P-512**

Material Chemistry

Event Hall THU 11:00~13:00

Thermal ammonolysis synthesis of molybdenum nitride layer on Mo foil and capacitor property

Dong Hyun Lim, Young-il Kim*

Department of Chemistry, Yeungnam University, Korea

Thin film layers of molybdenum nitrides (MoN_x) were grown directly on the molybdenum (Mo) foil by thermal ammonolysis at 1273 K for 2-20 h. Further, molybdenum dioxide (MoO_2) were obtained by heating the above MoN_x layer in the N_2 atmosphere. Scanning electron microscopy revealed a clear boundary between Mo and MoN_x layer, and the thickness of 200~700 nm of the latter. X-ray photoelectron spectroscopy showed that the binding energy of Mo 3d increased in the order Mo < MoN_x < MoO_2 < MoO_3. Electrochemical electrodes using the MoN/Mo foils and MoO_2/Mo foils show sufficiently low interfacial resistance and high stability in an aqueous acid condition. The capacitor properties were measured by cyclic voltammetry and galvanostatic charge-discharge in H_2SO_4.

Poster Presentation : **MAT.P-513**
Material Chemistry
Event Hall THU 11:00~13:00

Full-Day Electrocardiogram Monitoring for Multiple Days with Permeable Waterproofing Sensors

Joosung Oh, Yebin Park, Ik-soo Kim, Unyong Jeong*

Materials Science and Engineering, Pohang University of Science and Technology, Korea

The wearable healthcare patch is difficult to wear for multiple days due to the formation of sweat and water to monitor without detachment. The electrode with permeability and waterproofing can address the challenge. This study presents a stretchable and stable thin Au electrode that was fabricated by deposition on an imidized nanofiber mat. Since the external surface of the electrode is hydrophobic, while the contact surface is hydro-wetting, the porous electrode has excellent sweat permeability and waterproofing function concurrently. The electrocardiogram sensor using the electrode can monitor cardiac signals for 5 continuous days without detaching while performing various activities throughout the day, such as rest, exercise, shower, and sleep. This study proposes a modular setup of electrodes and cardiac signal processing unit to activate the device when cardiac monitoring is required.

Poster Presentation : **MAT.P-514**
Material Chemistry
Event Hall THU 11:00~13:00

SEAMLESS MONOLITHIC WATER SPLITTING SYSTEM USING MINIATURIZED CRYSTALLINE SILICON MICROWIRE INTERDIGITATED BACK CONTACT PHOTOELECTRODE

Wonjoo Jin, Kwanyong Seo*

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

We fabricated c-Si based wireless monolithic artificial leaf for an efficient unassisted photoelectrochemical water splitting (PEC). A seamless module was manufactured using a c-Si interdigitated back contact (IBC) structure. Through modularization, a photoelectrode having an overpotential of 1.5 - 2 V or more was realized. So unassisted water splitting was possible. We fabricated a c-Si IBC photoanode that obtained an efficiency of 10.1 % at 0 V (unassisted water splitting). An artificial leaf, an unassisted-wireless water splitting system, was fabricated using the proposed c-Si IBC solar cell and showed about 8.4 % STH, which was the highest performance among the reported silicon-based wireless PEC systems despite no optimization of catalysts. The design suitable for artificial leaf devices and the expectation of improved efficiency through the development of catalysts make the c-Si IBC module artificial leaf system promising for the unassisted photoelectrochemical hydrogen production in practical application.

Poster Presentation : **MAT.P-515**

Material Chemistry

Event Hall THU 11:00~13:00

Size-dependent adsorption of DNA on layered double hydroxides

Jing Xie, **Jae-Min Oh***

Department of Energy and Materials Engineering, Dongguk University, Korea

Layered double hydroxides (LDHs) with different particle diameters were synthesized, and its adsorption behavior of deoxyribonucleotide (DNA) was examined with respect to the strand length of DNA. Small-sized LDH (LDH-S) was synthesized by conventional coprecipitation by titrating the mixed metal solution with an alkaline solution until pH of ~9.5; while large-sized particle (LDH-L) was prepared by urea hydrolysis method. The X-ray diffraction patterns indicated that the LDH-L had higher crystallinity than the LDH-S, and the scanning electron microscope showed average particle diameters of 20 nm and 2500 nm, for LDH-S and LDH-L, respectively. Adsorption isotherm of genomic DNA with a wide range of lengths illustrated that LDH-S had a good agreement with Freundlich model, describing multilayered-adsorption. On the other hand, the isotherm of LDH-L followed Sips model, depicting a combination of single-layer and multilayer adsorption. The electrophoresis of ladder DNA after adsorption revealed that DNA with less than 800 bp length was more adsorbed by LDH-S than LDH-L. On the contrary, long-stranded DNA (>800 bp) was more effectively adsorbed by LDH-L than LDH-S. Consequently, the large particle size of LDH tended to adsorb long DNA strands, and the small particle size of LDH inclined to adsorb a shorter DNA.

Poster Presentation : **MAT.P-516**

Material Chemistry

Event Hall THU 11:00~13:00

Biocompatibility of drug intercalated layered double hydroxide to plasma protein and blood cells

Jing Xie, Jae-Min Oh*

Department of Energy and Materials Engineering, Dongguk University, Korea

Anticancer drug methotrexate (MTX) was intercalated into layered double hydroxide (LDH), and the hematocompatibility of the hybrid (MTX-LDH) was evaluated based on the biological behavior of hybrid toward plasma protein and blood cell. The X-ray diffraction pattern on synthesized MTX-LDH showed that MTX molecules were arranged in a slightly tilted configuration between LDH nanosheets. The scanning electron microscope presented that the average particle size of MTX-LDH was 120 nm with narrow size distribution. The negative zeta potential of the hybrid (□17.0 mV) slightly shifted to a positive (+7.6 mV) region, and the large hydrodynamic radius (> 1000 nm) became small upon incubating with plasma for 6 h. The result suggested the high dispersibility of MTX-LDH hybrid under physiological fluid, probably due to the protein corona formation at the surface of MTX-LDH. The MTX drug alone readily quenched fluorescence of protein under plasma state, showing0.99 of quenching ratio at 0.4 mg-LDH/mL concentration. On the other hand, the fluorescence quenching ratio of MTX-LDH was saturated at around 0.95 at 1.5 mg-LDH/mL. The results implied that the strong protein-MTX was effectively blocked by the LDH. The quartz microbalance assay revealed that MTX-LDH could reversely adsorb and desorb albumin upon proteins solution and deionized water treatment. The in vitro hemolysis assay after mixing MTX-LDH and human blood was 2.66 % at 10 mg-LDH/mL for 0.5 h, which was in the permissible range of hematocompatibilty. The scanning electron microscope of blood after MTX-LDH administration did not show serious conformation change of blood cells, while some MTX-LDH particles were found at the surface of red blood cells. It could be concluded that the MTX-LDH hybrid was highly compatible with blood components by forming protein corona at the surface and by attaching to the blood cell through non-covalent interaction.

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Poster Presentation : **MAT.P-517**
Material Chemistry
Event Hall THU 11:00~13:00

Ammonolysis synthesis of titanium nitride layer on Ti foil and supercapacitor property

Songhyeon Kim, Young-il Kim*

Department of Chemistry, Yeungnam University, Korea

Titanium nitrides were synthesized by thermal ammonolysis of titanium foil in ammonia atmosphere at 1173-1273 K and for 2-20 h. According to the powder X-ray diffraction analysis, titanium (hexagonal) transforms to Ti_2N (trigonal) at 1173 K and then to TiN (cubic) at higher temperatures. Upon the ammonolysis of Ti, the mass increased by 1~10 % depending on the time and temperature of ammonolysis, which correspond to the fraction of 10 - 25% for titanium nitride in the final foil. Impedance analysis showed that the titanium nitride layers possess conductivities of ??~?? S/cm, giving promises as electrochemical electrodes. Pseudo-capacitor behavior of titanium nitride layers were investigated by cyclic voltammetry and galvanostatic charge-discharge in acidic (1 M H_2SO_4) and basic (1 M KOH) media.

Poster Presentation : **MAT.P-518**

Material Chemistry

Event Hall THU 11:00~13:00

2D Holey Nickel Cobalt Mixed-Oxide Nanosheets for Lithium-Ion Batteries: via Dimensional-Confined Solid-State Conversion

Yu-Rim Hong, Byeongsu Gu, In Su Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Two-dimensional (2D) nanomaterials are attracting great attention in the field of next-generation energy storage and conversion devices because of their confined thickness and large exposed surface area. However, the fabrication of atomically thin 2D nanomaterials by facile routes still remains a big challenge. This study proposes a dimensional-confined solid-state conversion strategy using layered double hydroxide (LDH) and silica nanoshell for preparing of ultrathin holey NiO-CoO mixed-oxide nanosheets. The 2D holey structure particularly designed may increase a contact interface between electrode and material, endure a volume change of electrode for a cycle, and improve electrochemical performance by shortening a Li^+ ions diffusion path. The thin NiO-CoO nanosheets of 1 nm are used as an anode material for a lithium-ion batteries (LIBs), exhibiting high reversible lithium storage capacity, long cycling stability (792 mA h g^{-1} after 450 cycles at 1788 mA g^{-1}), and durable high-rate capability (400 mA h g^{-1} after 1000 cycles at 4470 mA g^{-1}). The reported simple manufacturing method utilizing dimensional-confined strategy provides a way for the design and massive production for 2D electrode nanomaterials for high-performance LIBs.

Poster Presentation : **MAT.P-519**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation of Lignin-polymer nanofiber composite membranes by electrospinning method

Dasol Jin, Eun-Bum Cho*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Lignin is a lignocellulosic biomass and is a biodegradable natural polymer derived from nature. In this study, we present a simple method for making nanofibers through electrospinning to apply lignin as a biomaterial with high added value. Alkalized kraft lignin and polyacrylonitrile (PAN) were used as basic polymers for composite nanofibers. The mixing ratio was 10 wt% of the total polymer content compared to the solvent DMF, and the mixing weight ratio was gradually increased from 1:9 to 3:7 based on Lignin:PAN. In addition, nanofibers were additionally obtained by electrospinning together with PAN in the same ratio using the modified material by esterification of lignin. Structural morphology was confirmed through HR-SEM (High Resolution Field Emission Scanning Electron Microscope), and physicochemical properties of nanofibers were analyzed through FT-IR and TGA. Polyacrylonitrile is a multi-purpose polymer used in various products such as filtration membranes and carbon fibers. Nanofibers spun together with PAN and lignin are expected to be biodegradable and eco-friendly materials with various applications such as storage and filtration.This study was supported by the Human Resource Developement Programs for Green Convergence Technology funded by the Korea Ministry of Environment(MOE).

Poster Presentation : **MAT.P-520**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation of hollow mesoporous silica nanospheres using pentablock copolymer templates containing Rhodamine B fluorescent dye

Jae Won Jo, Eun-Bum Cho*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Pluronic copolymers are a kind of amphiphilic and biocompatible block copolymers and it has effectively been applied as a carrier for drug delivery. In order to exploit micellar morphology of modified block copolymer, we synthesized PLGA-PEO-PPO-PEO-PLGA pentablock copolymers by attaching a biodegradable PLGA block at the both ends of a pluronic triblock copolymer. Hollow mesoporous silica nanospheres were prepared using organosilica precursor and a PLGA-PEO-PPO-PEO-PLGA pentablock copolymer as a template. In this study, RhB was introduced into the hydrophobic moiety of the block copolymer chains to prepare fluorescent nanospheres. Systematic characterization of the sample was performed by using TEM, SEM, confocal microscopy, and UV absorbance. From the result, fluorescent nanospheres can be prepared in one-pot process and the application for biomedical/chemical fluorescent sensors is expected.This study was supported by the Human Resource Development Programs for Green Convergence Technology funded by the Korea Ministry of Environment(MOE).

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Poster Presentation : **MAT.P-521**

Material Chemistry

Event Hall THU 11:00~13:00

A Study on the Combustion Characteristics of Magnesium Powder using Optical and FE-SEM Analysis

Songyi Han, Junsik Lee*

Department of Aeronautical & Mechanical Engineering, Changshin University, Korea

Magnesium is being used extensively in military aeronautics, chemical and metallurgical industries. However, magnesium is a representative combustible metal that easily reacts with oxygen and nitrogen has a very high risk of fire and explosion. In this experiment, magnesium powder was burned by raising the temperature to 700°C using a controller and an ignition equipment. The magnesium powder with the purity is 99% or more(purity > 99%) used in this study is 75µm, 100µm, and 150µm, respectively. An optical microscope and a field-emission scanning electron microscope (FE-SEM) were used to confirm particle properties. It concludes the significant tendency of magnesium fire, combustion products' particle characteristics.key word : Magnesium powder, Combustible metal, Optical microscope, FE-SEM

Poster Presentation : **MAT.P-522**

Material Chemistry

Event Hall THU 11:00~13:00

Silica Nanoreactor with Chemo-Enzymatic Compartments for Enantioselective Synthesis inside Living Cells

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Department of Chemistry, Pohang University of Science and Technology, Korea

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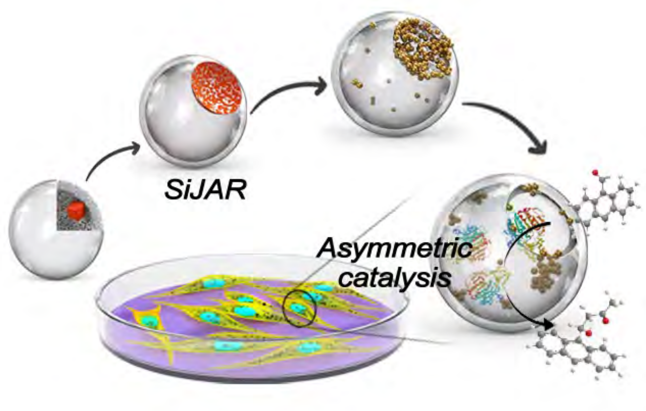
Chemical reactions are regulated by the presence of organelles or core structures of cells that accommodate specific enzymes or cofactors. A nanoreactor with both the activity of a synthetic catalyst, such as an artificial organelle that mimics a cell, and the properties of an enzyme creates a platform for selectively synthesizing natural enantiomeric bioactive molecules that can respond to pathogens – such as drugs – in the body. However, until now, a nanoreactor with the functions of both a synthetic catalyst and an enzyme for such a platform has not been reported. Here, we synthesized silica nanostructures (SiJARs) such as round-bottom jars with chemically reactive metal-silicate lids via solid-state nanocrystal conversion, the subsequent galvanic replacement and followed by the enzyme encapsulation. SiJARs performed asymmetric aldol reactions with high activity and enantio-selectivity (yield >99%, ee = 95%, and also functioned as an artificial catalytic organelles inside living cells. The hybrid chemoenzymatic nanodevice, customizable through this sophisticated solid-state conversion strategy, can be utilized for synthesizing active therapeutics and bioimaging probes locally inside cells to be suitable for use in next generation bioimaging and treatment.


SiJAR
Asymmetric catalysis

Poster Presentation : **MAT.P-523**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of Mixed-Dimensional In-Plane Heterostructures Composed of Monolayer MoS_2 and Low-Dimensional Mo/Te compounds

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Energy Systems Research, Ajou University, Korea
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Mixed-dimensional heterostructures formed by combining 2D materials and other dimensional (0D, 1D, and 3D) materials have new opportunity for various applications due to their novel structures. Here we report a novel chemical vapor deposition method for synthesizing in-plane heterostructures consisting of monolayer MoS_2 and low-dimensional Mo/Te compounds. . The composition and phase of the low-dimensional Mo/Te compounds interfaced with MoS_2 are controlled by the Te flux and growth time. At low Te flux, in-plane 2D/1D MoS_2/Mo_6Te_6 and 2D/2D/1D MoS_2/2H $MoTe_2/Mo_6Te_6$ heterostructures are selectively obtained depending on the growth time. While at high Te flux, in-plane 2D/2D MoS_2/mixed 2H-1T' $MoTe_2$ and 2D/2D MoS_2/2H $MoTe_2$ heterostructures are selectively synthesized depending on the growth time. The Te flux-controlled method will broaden the possibility for the synthesis of mixed-dimensional in-plane heterostructures.

Poster Presentation : **MAT.P-524**

Material Chemistry

Event Hall THU 11:00~13:00

Purification of plasma BNNTs and optical analysis in each process

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BNNT is a material attracting attention in aerospace engineering due to its excellent thermal and chemical stability and thermal neutron shielding properties. As a result of thermal plasma synthesis, which is currently capable of mass synthesizing BNNT at a rate of 20 g/h, impurities other than BNNT (e.g., amorphous boron, a-BN, BN shell, BN flakes) are observed in the final product. Since these impurities are an obstacle in the study of BNNT applications, a purification process to remove impurities from the synthesized BNNT samples seems to be necessary. In this study, the amorphous boron in the synthesized plasma BNNT was oxidized with B_2O_3 in a furnace at 650 °C and dissolved in water to remove it. Impurity BN was removed by repeatedly filtering through a 35 um pore mesh using a smaller aspect ratio than BNNT. Oxidized Boron (B_2O_3) appeared in Raman, IR, and the signal disappeared after dissolution, suggesting that B_2O_3 was successfully removed. Removal of BN material with low aspect ratio was shown to decrease FWHM of E_{2g} mode in Raman and decrease in intensity of radial buckling mode (R) compared to transverse optical mode (TO) intensity in IR. Impurities were reduced in plasma BNNT, and the purification efficiency could be assessed through optical analysis.

Poster Presentation : **MAT.P-525**
Material Chemistry
Event Hall THU 11:00~13:00

Synthesis of boron nitride nanotubes via metal-catalytic arc discharge using molecular precursor

Juseong Park, Myung Jong Kim*

Department of Chemistry, Gachon University Global Campus, Korea

Arc discharge, which is one of the methods for synthesizing BNNTs, causes continuous electron-gas molecular collisions due to thermionic emission from the cathode and the formation of an electric field between the cathode and anode. The arc discharge method has the advantage of good crystallinity because it is a method under high temperature conditions of about 3000~5000K, but it has the disadvantage of very low electrical conductivity due to the property of the metalloid of boron. In a previous study, an experiment was conducted by overcoming the disadvantages by using a boron-containing anode with a small amount of metal added to the anode. In this experiment, B and N were supplied by using tungsten as an electrode and borazine(carrier gas H_2) gas as a precursor. Experimental results were analyzed by SEM, TEM, EDS, and Raman. SEM and TEM confirmed that the growth of BNNT was tip-growth, and EDS-mapping confirmed that catalyst was contained in the tip. In Raman analysis, a sharp 1370cm^{-1} peak of E_{2g} was observed. By using tungsten anode to stably maintain arc plasma, the disadvantages of arc discharge BNNT synthesis were compensated. Also, I think that it is a method to improve the efficiency by converting from the solid precursor to the molecular precursor borazine.

Poster Presentation : **MAT.P-526**

Material Chemistry

Event Hall THU 11:00~13:00

Alternative synthesis of BNNTs or BN-MgO core/shell nanowires by CVD

Chunghun Kim, Myung Jong Kim[1,*]

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Although BNNT is a new material attracting attention for its excellent mechanical properties, excellent heat resistance, high thermal conductivity, insulation, and radiation shielding, it has been mainly synthesized through high-temperature and high-energy methods such as laser ablation and plasma methods. CVD synthesis using a supported catalyst is a method with the potential to mass-synthesize BNNTs at low temperatures. In this study, we report that pure BNNT and BN-MgO core/shell nanowires were synthesized by controlling the degree of oxidation of MgO used as a support for a metal catalyst. By controlling the synthesis conditions, it was possible to control the length of the BN-MgO core/shell nanowire and the thickness of the BN shell. The crystallinity of the synthesized BNNT and BN-MgO core/shell nanowire was confirmed using transmission electron microscopy and XRD, and thermal stability was evaluated through TGA analysis. The synthesized BN-MgO core/shell nanowire has high thermal stability and neutron shielding properties, suggesting that it can be applied to space materials. In addition, only BN fibers were obtained by removing only MgO from the BN-MgO core/shell nanowire through simple acid treatment. Although the obtained BN fiber has similar properties to BNNT, it is relatively easily synthesized and can be synthesized in large amounts, so its application through compounding with other materials is expected.

Poster Presentation : **MAT.P-527**
Material Chemistry
Event Hall THU 11:00~13:00

BNNT purification and length fractionation by gel column chromatography

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[1]*nanochemistry, Gachon University Global Campus, Korea*

BNNTs have excellent insulating properties, effective neutron shielding, and high thermal conductivity. These characteristics can be applied to various industries such as the space industry using dielectric and neutron shielding of electronic products. However, the low BNNT synthesis yield of under 50% caused by impurities such as h-BN makes it difficult to implement in practical applications. Here we present the purification and length fractionation of these mixtures via gel column chromatography. During the chromatography process, BNNTs are effectively separated according to the difference in their affinity for the gel. This is used to classify by length, and the length for each chromatographic section is suggested through the SEM image. The removal of amorphous boron, h-BN, is demonstrated by FTIR and Raman analysis of purified BNNT samples. The 1367 cm^{-1} peak of BNNT E_{2g} in Raman shows a decrease in FWHM after purification. Similarly, the sharpness of the peaks of LO and RO modes of BNNTs appearing at 1400 cm^{-1} and 750 cm^{-1} in FTIR and removal of 3200 cm^{-1} of B_2O_3 means that the purification of BNNTs is achieved through gel chromatography. We believe that high-purity BNNTs with these customized nanotube lengths provide suitable properties for BNNT applications and are a practical way to prepare pure BNNT dispersions of desired lengths.

Poster Presentation : **MAT.P-528**
Material Chemistry
Event Hall THU 11:00~13:00

Ethyleneamines-functionalized metal-organic framework, MOF-808: Selective adsorbent to capture CO_2 under low pressure

HyeokJoon Jun

Department of Chemistry, Kyungpook National University, Korea

A metal-organic framework (MOF) prepared from Zr and 1,3,5-benzenetricarboxylic acid, MOF-808, was functionalized with ethyleneamines such as tetraethylenepentamine (TEPA), diethylenetriamine (DETA), and ethylenediamine (ED) to utilize the obtained MOFs in selective capture of CO_2 from offgas under low pressure. The modification was done firstly in the liquid phase via an acid-base reaction (using μ-OH of the MOF), and TEPA was the most effective among the tested ethyleneamines because of the low basicity of the TEPA. MOF-808s functionalized with TEPA were very efficient in CO_2 capture because of loaded primary and secondary amino groups. For example, one MOF-808, functionalized with an adequate quantity of TEPA, showed remarkable performances in CO_2 adsorption with a very high ideal adsorption solution theory selectivity of 256 which is around 7 times that of the pristine MOF-808. Moreover, the modified MOF-808 adsorbed around 2.5 times CO_2 that of the pristine M-808 at 15 kPa. The noticeable performance of the functionalized MOF-808 was explained with the loaded amino groups that are capable of a Lewis acid-base interaction with CO_2 to form carbamates. This work will pave the way to modify a MOF, although without open metal sites, to introduce amino groups that will be very effective in selective capturing of CO_2 from offgas.

Poster Presentation : **MAT.P-529**

Material Chemistry

Event Hall THU 11:00~13:00

Nanogap-Enhanced Raman Scattering in Solution as a Highly Sensitive and Reproducible Assay Platform for Bacterial Genome Detection

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KU-KIST Graduate School, Korea University, Korea
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Surface-enhanced Raman scattering (SERS) has been investigated as a promising spectroscopic tool for various assay platforms. However, key challenges, such as reproducibility and sensitivity, need to be overcome for SERS to become a reliable and practical method for future clinical applications. There is an unavoidable tradeoff between the signal reproducibility and sensitivity of the SERS-based assay, especially in a dry-state analytical condition. The signal reproducibility can be significantly improved by obtaining the Raman signal from the solution state. In this work, we report a highly sensitive solution state SERS-based nucleic acid detection method using a solution-state formation strategy of gold-silver core-shell nanodumbbells (GSNDs); the GSNDs induced significantly enhanced Raman signal intensity. The yield of dimeric nanostructures with target nucleic sequences is linearly correlated to the amount of target nucleic acid. Diverse parameters like the length of target sequences, hybridization conditions and kinetics, and oligonucleotide sequences were investigated. To envision the potential of the solution-state GSND-based assay, new nucleic acid target sequences for five different bacteria—*Escherichia coli*, *Enterococcus faecalis*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*—were selected and confirmed. The key parameters affecting the assay results are systemically investigated in this study. We found that the solution-state GSND-based assay showed a femtomolar or attomolar sensitivity for bacterial target DNA without any interference among them, which indicates a strong potential of the assay to detect nucleic acid targets of interest.

Poster Presentation : **MAT.P-530**

Material Chemistry

Event Hall THU 11:00~13:00

Bi-metallic nanoparticle catalyst synthesis for BNNT or CNT growth

Minseo Kim, **Myung Jong Kim***

Department of Chemistry, Gachon University Global Campus, Korea

Metal nanoparticles have been widely applied in various commercial fields. Nanoparticles have a large effect on specific activity depending on their size, so it is important to synthesize small-sized particles. Among many different methods for the synthesis of nanoparticles, the reverse micelle method is most widely used nowdays because the size of the particles can be easily adjusted with nanosized aqueous droplets existing at certain compositions of water-in-oil microemulsions. By using the protective agent of DDAB, Ni-Pd nanoparticles were successfully synthesized. Through the analysis by transmission electron microscope (TEM), the synthesized particles were confirmed to have an average diameter in the range of 2.0-4.0 nm depending on the size distribution, and the particle lattice structure was observed through HRTEM. The energy dispersive X-ray spectroscopy (EDS) mapping was applied to identify the composition and the alloy formation of the Ni-Pd bimetallic nanoparticles. As a result, the Ni-Pd particles were successfully synthesized by composing Ni and Pd elements. Homogeneous and polymer-stabilized Ni-Pd bimetallic nanoparticles were applied as catalysts to grow CNTs/BNNTs.

Poster Presentation : **MAT.P-531**

Material Chemistry

Event Hall THU 11:00~13:00

Humidity sensing character of carboxylated multiwall carbon nanotubes based sensor; simple and easy detection of relative humidity

Sangmin Kim, Jihyeon Mun, Jiyeong Park, Songmi Bae, Don Kim*

Department of Chemistry, Pukyong National University, Korea

Carboxylated and biochemically-modified multiwall carbon nanotubes (MWCNTs) based humidity sensor for the detection of relative humidity (RH%) in air was demonstrated. The modified MWCNTs was deposited on interdigitated gold electrode (10 ㎛ gap with 60 fingers) and on microfilter paper. The sensitivity was expressed by relative resistance change (RH_S(%) = (R_{meas}-R_{dry})/(R_{wet}-R_{dry}) x 100), where R_{meas} is the resistance of under test, R_{wet} is the resistance under RH% = 83, and R_{dry} is the resistance under dry N_2 flow (RH% = 3). The interaction between carboxyl group on the modified MWCNTs and water vapor will cause the electron donating from water molecules to MWCNTs. At high humidity, the resistance of the sensor increased 20% from RH(%) = 3 to RH(%) = 83. Also the potential barrier between MWCNTs was increased by the water adsorption at high water vapor pressure. The sensor shows faster detection speed (< 45 s) than a commercial sensor (~65 s).

Poster Presentation : **MAT.P-532**

Material Chemistry

Event Hall THU 11:00~13:00

Cationic Promotion of H_2O_2 Electrosynthesis Activity of O-Doped Carbons

Juyeon Lee, Young Jin Sa*

Department of Chemistry, Kwangwoon University, Korea

H_2O_2 electrosynthesis is an emerging clean chemical technology, whose efficiency critically depends on the activity and selectivity of electrocatalysts for two-electron oxygen reduction reaction ($2e^-$ ORR). In this presentation, it is demonstrated that $2e^-$ ORR activity of oxygen-doped carbons, which have been one of the most promising catalysts for this reaction, can be substantially influenced by the types and concentrations of cations in electrolytes. Heat-treated carbon comprising active oxygen functional groups exhibits cation-dependent $2e^-$ ORR activity trends in alkaline media, following the order $Cs^+ > K^+ > Li^+$. Importantly, an electrolyte with a high cation concentration (0.1 M KOH + 0.5 M KCl) afforded the highest $2e^-$ ORR mass activity (250 ± 30 A g_{cat}^{-1} at 0.70 V vs reversible hydrogen electrode) ever reported. It was revealed that the cation promotion effect correlates with cation-dependent electron-transfer kinetics, which regulates the rate-determining first electron transfer to O_2.

Poster Presentation : **MAT.P-533**

Material Chemistry

Event Hall THU 11:00~13:00

Improvement of the Electrode Performance of Prussian Blue Analogues via the Hybridization with Ruthenium Oxide Nanosheets

Yoon Chang Hong, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

An effective way to explore high performance electrode for Na-ion batteries is developed by employing exfoliated inorganic nanosheet as an immobilization matrix for Prussian blue (PB) nanocrystals. The intimately-coupled nanocomposites of Mn-Ni-PB-RuO_2 NS (MNPBR) are synthesized by crystal growth of Mn-Ni-PB nanocrystals on the exfoliated RuO_2 nanosheets. The obtained MNPBR hybrid shows higher cathode performance with better electrochemical stability than the pristine MNPB, confirming the beneficial effect of hybridization on the electrode performance and stability of PB. The present results confirm that RuO_2 NSs can work as an effective conductive additive for electrode materials by stabilizing the crystal structure during intercalation/deintercalation processes and by enhancing charge transfer properties between hybridized species.

Poster Presentation : **MAT.P-534**
Material Chemistry
Event Hall THU 11:00~13:00

CONTROLLING ACID SITES OF MIXED METAL OXIDE STARTING FROM LAYERED DOUBLE HYDROXIDE WITH VARIOUS MG/AL RATIO Vidya Chandrabose, Jae - Min Oh

Jae-Min Oh*, Chandrabose Vidya[1]

Department of Energy and Materials Engineering, Dongguk University, Korea
[1]*Energy And Materials Engineering, Dongguk University, Korea*

ABSTRACT CONTROLLING ACID SITES OF MIXED METAL OXIDE STARTING FROM LAYERED DOUBLE HYDROXIDE WITH VARIOUS MG/AL RATIO Vidya Chandrabose, Jae - Min Oh Department of Energy and Materials Engineering, Dongguk University, Seoul, 04620, Republic of KoreaMixed metal oxides (MMO) have attracted increasing interests in the development of heterogenous catalysis due to its active acidic or basic sites, redox properties porosity and huge specific surface area. In this study, MMO was synthesized by the calcination of layered double hydroxides which was prepared by conventional coprecipitation method. In order to control acid sites in MMO, Mg/Al molar ratio in starting LDH was set in four different values. X-ray diffraction analysis confirmed that all the four MMO consisted of typical periclase structure with comparable crystallinity. The Mg/Al ratio of the four MMO was determined 1.01, 2.01, 2.98, 4.14 based on inductively coupled plasma-optical emission.. Specific surface area values of MMOs were not significantly different from each other ranging between 100-200 m2/g (125.7, 173.8, 139.78, 134.65 m2/g, for Mg/Al ratio 1.01, 2.01, 2.98, and 4.14, respectively). The degree of acid site was investigated by monitoring temperature programmed desorption of ammonia, suggesting that highest physisorption affinity was showed by MMO with Mg/Al ratio 4.14; however, strong chemisorption was observed in MMO with Mg/Al ratio 1.01.

Poster Presentation : **MAT.P-535**

Material Chemistry

Event Hall THU 11:00~13:00

Simple sequential deposition method for the efficient multi-component organic solar cells without the complex optimization steps

YoungWoo Kwon, Doo-Hyun Ko*

Department of Chemistry, Sungkyunkwan University, Korea

Multi-component bulk-heterojunction (BHJ) systems could provide an opportunity to fabricate organic photovoltaic cells (OPVs) that achieve high power conversion efficiency. However, as the involving element increases in the BHJ system, the journey to finding optimal experimental conditions in the fabricating step becomes more complicated. Here, we propose the sequential deposition approach that does not go over the conventional complex optimization process. Modified quaternary BHJ system was built by sequentially depositing the two binary donor:acceptor blends. By using well-known and optimal binary blends, it was more facilitated to reduce the experimental factors required for the optimization of the quaternary system than that of the conventional system. Surprisingly, the altered quaternary BHJ layer showed ameliorated device performance through the optoelectronic advantages provided by the two binary blends and optimal film morphology. Spontaneous molecular arrangement and blending occurred during the sequential process, which was facilitated to build effective cascade energy level alignment in the quaternary BHJ system. The universality test was performed to apply for the various BHJ layers, and our processing strategy also worked well in extended blend systems. The alternative sequential deposition methodology suggests a new opportunity to overcome the existing shortcomings for high-performance BHJ OPVs.

Poster Presentation : **MAT.P-536**

Material Chemistry

Event Hall THU 11:00~13:00

Non-fullerene organic photovoltaics enabled for efficient photon harvesting under indoor lighting environments

Gyu-Hee Kim, Doo-Hyun Ko[1,*]

Chemistry, Sungkyunkwan University, Korea

[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Organic photovoltaics (OPVs) have attracted lots of attention as an indoor power generation application for the Internet of Things. In this study, the high-performance non-fullerene OPVs are demonstrated at various environments through a high understanding for the origins of efficient operating mechanisms depending on illuminance. Compared to the fullerene OPVs, the non-fullerene OPVs show higher performance under various indoor lighting environments, despite the mismatching of the irradiance spectrum. The non-fullerene systems exhibit morphological characteristics as nanoscale phase separation between each component, resulting in building the effective charge transport pathway. These morphological features are associated with ameliorated charge recombination, leading to restrained voltage loss. That is, this study suggests a direction for the advantageous morphology that an ideal bulk hetero-junction OPV should pursue under a variety of indoor irradiation conditions.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-537**

Material Chemistry

Event Hall THU 11:00~13:00

Efficient Light Trapping Film for Operable Semitransparent Photovoltaics in Outdoor and Indoor Environment

Jung-Hyun Lee, Doo-Hyun Ko*

Department of Chemistry, Sungkyunkwan University, Korea

Efficient light-trapping polymer films are introduced to improve the photocurrent generation of semitransparent organic photovoltaics (ST-OPVs) in indoor and outdoor conditions. An asymmetric-reflection film featuring arranged nanostructures with assembled microstructures exhibits selectivity for the direction of incident light, thus efficiently trapping light within the device. The film is attached to the double-sided ST-OPV operating simultaneously under solar and indoor light sources, that can be operated to maximize the effect of capturing light. These light-trapping platforms show the short-circuit current density enhancements of ST-OPVs by 13.49% and 46.19% under 1 sun AM 1.5 G and light-emitting diodes (1000 lux) illumination.

Poster Presentation : **MAT.P-538**

Material Chemistry

Event Hall THU 11:00~13:00

Enhanced Photoluminescence of CsPbX3 PNCs via Monolithic CsPbX3-SiO2 Nanopatterns and their Application

YongJae Cho, Doo-Hyun Ko*

Department of Chemistry, Sungkyunkwan University, Korea

We propose a simple yet effective strategy via the incorporation of CsPbX3 perovskite nanocrystals (PNCs) with SiO2 nanopatterns. The fabrication process of CsPbX3-SiO2 nanopatterns is containing the nano-imprinting lithography and thermal curing of perhydropolysilazane (PHPS) polymer precursors of SiO2 crystals. The prepared various CsPbBr3-SiO2 nanopatterned films show the significantly amplified photoluminescence (PL) intensities as up to 4.62 times compared to the planar counterpart, maintaining the high transparency over 90% at the visible region. The CsPbBr3-SiO2 film efficiently converts incident blue light of light-emitting diode (LED) to green light with high conversion yields (72.3%). The time-resolved PL analysis and finite-difference time domain (FDTD) calculations infer that the enhanced PL performances are derived from Mie scattering resonance at excitation and emission wavelengths. We further fabricate the vivid multi-colored picture by modulating the proportion of halide composites in the CsPbX3 PNCs (red: CsPbBr0.9I2.1, green: CsPbBr3, blue: CsPbCl1.2Br1.8). Through the considerably enhanced optical performances of the CsPbX3 PNCs, this approach can sufficiently extend their potential for display devices with a wide color gamut.

Poster Presentation : **MAT.P-539**

Material Chemistry

Event Hall THU 11:00~13:00

Essential Electron Transport Layer For Highly Efficient Organic Photovoltaics Under Indoor Conditions

Hyeon-Yeong Jo, Doo-Hyun Ko*

Department of Chemistry, Sungkyunkwan University, Korea

Organic Photovoltaics (OPV) has been attracting attention due to its excellent stability. For reverse OPV, metal oxides and conjugated polyelectrolytes as electron transport layers (ETLs) have been extensively used to enhance charge collection. However, since the operating mechanism of OPV varies according to the amount of light, it is required to recognize the function of ETL according to the amount of light. The good ETL material provides effective charge transporting, charge selectivity and reduces the shunt resistance to prevent recombination. Unlike the OPV performance of the two ETLs (ZnO and PFN-Br) , which were similar in 1-sun irradiation, they are different in low light irradiation. We confirm that ZnO operates better performing OPVs in low-light lighting, including indoor conditions. The use of ZnO ETL assures high photovoltaic performance in low-light irradiation environments and facilitates photovoltaic cell fabrication through simple single ETL deposition process. Therefore, ZnO can achieve high-efficiency OPV in low-light lighting including indoor conditions.

Poster Presentation : **MAT.P-540**

Material Chemistry

Event Hall THU 11:00~13:00

Enhanced upconversion photoluminescence by quasi-periodic metal-insulator-metal (MIM) platform and photochemical switching application

<u>Chi Hyung Lee</u>, Doo-Hyun Ko[1,*]

Department of chemistry, Sungkyunkwan University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Photo-switchable upconversion nanoparticles (UCNPs) have considerable attention due to their unique optical characteristics, which exhibits different photoluminescence (PL) spectra depending on the incident power intensity. In this study, we propose an effective strategy for enhancing photoswitchable upconversion PL (UCPL) by introducing quasi-periodic metal nanopatterns–insulator–metal (MIM) platform. A quasi-periodic metal array was elaborately incorporated by sequential rotating metal-transfer lithography onto the UCNP-embedded SiO2/Ag substrate. With the quasi-periodic MIM structure, PL intensities were significantly amplified over two-orders degrees, maintaining the spectral orthogonality. The time-resolved PL and calculated electric field distribution profile supported that the PL enhancement is induced by amplified plasmonic mode of quasi-periodic metal array. Finally, we validated that our developed platform can elicit effective photochemical light trigger with the accelerated photoisomeric kinetics and significant photo-fatigue resistance.

Poster Presentation : **MAT.P-541**
Material Chemistry
Event Hall THU 11:00~13:00

Selectively Synthesized Monolayer and Spiral Few-Layer $MoSe_2$ by Flux-Controlled Chemical Vapor Deposition

JooHyeon Ahn, Youngdong Yoo[1,*]

Department of Energy System Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

Transition metal dichalcogenides (TMDCs) have been extensively utilized as advanced materials for various applications. Monolayer TMDCs have been used for flexible optoelectronics and 2D electronics due to their atomically thin layered structure and physical and chemical properties. Spiral TMDCs have been used for various nonlinear optical applications due to their unique optical properties. However, the selective synthesis of monolayer and spiral TMDCs is quite challenging. Here we report that we selectively synthesized monolayer and spiral $MoSe_2$ on face-up SiO_2/Si substrate by a flux-controlled chemical vapor deposition method using both $MoSe_2$ powder and NaCl powder. Monolayer $MoSe_2$ was synthesized when the $MoSe_2$ flux was low, whereas few-layer spiral $MoSe_2$ was obtained when the $MoSe_2$ flux was high. As-synthesized monolayer and few-layer spiral $MoSe_2$ were characterized through optical microscopy, Raman and photoluminescence spectroscopy, atomic force microscopy, and power-dependent second harmonic generation measurements. We believe our method developed here can be generally applicable to selective growth of other monolayer and spiral TMDCs.

Poster Presentation : **MAT.P-542**

Material Chemistry

Event Hall THU 11:00~13:00

Crystal Structure Dependence of Photochromism of Nanocrystalline WO_3 and MoO_3 Prepared by Temperature-Controlled Acid-Precipitation Method

Young Hee Jung, Yeong Il Kim[1,*]

Research & development center, Adchro, Korea

[1]*Department of Chemistry, Pukyong National University, Korea*

Photochromism is a very useful property for modulating solar radiation. Two types of photochromic materials have been widely investigated: organic materials and inorganic transition metal oxides. Although organic photochromic materials exhibit relatively large modulation and fast response, their lack of durability makes them less useful from a practical point of view. The transition metal oxides such as WO_3, MoO_3, Nb_2O_5, V_2O_5 and TiO_2 exhibit photochromism by band gap irradiation. Their photochromic characteristics are so widely variable depending on crystal size, structure, morphology and impurities. Among the photochromic transition metal oxides WO_3 and MoO_3 have been studied most extensively. Nevertheless, their photochromic properties have still not been clearly characterized. We have synthesized three different crystal structures of nanocrystalline WO_3 and MoO_3 by temperature-controlled acid precipitation of their polyoxometalate. Their photochromic characteristics are comparatively investigated in this study.

Poster Presentation : **MAT.P-543**

Material Chemistry

Event Hall THU 11:00~13:00

Ionic conductivity of rock-salt Li_3TaO_4 depending on polymorphism and defect type

Chaeeun Kim, Young-il Kim*

Department of Chemistry, Yeungnam University, Korea

Ionic conductivity of complex rock-salt Li_3TaO_4 was studied using high-temperature (LTOH) and low-temperature (LTOL) polymorphs and with interstitial or vacancy defects. For each of LTOL and LTOH derivatives, four samples were prepared with different nominal compositions of $Li_{3.05}Ta_{0.99}O_4$ (LTO_3.05L/H), Li_3TaO_4 (LTO_3.00L/H), $Li_{2.99}Ta_{1.002}O_4$ (LTO_2.99L/H), $Li_{2.98}Ta_{1.004}O_4$ (LTO_2.98L/H). The synchrotron X-ray Le Bail refinement showed that the ordered LTOH phases have greater lattice volume than the disordered LTOL phases. Among both LTOL and LTOH sample groups, the lattice volume was smallest for the stoichiometric phases LTO_3.00L/H. The Li-7 solid-state magic angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy indicated that there exist two distinct chemical environments for Li in all samples. According to the AC impedance measurement and equivalent circuit analysis, both the vacancy and interstitial-type defects contributed to increase the ionic conductivity of LTO_3.00L/H and to similar extents.

Poster Presentation : **MAT.P-544**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation and Characterization of Biodegradable PLA/PCL Blending Chips.

Sung Hwa Oh*, Seung Hyuck Bang[1], Yuseon Noh[2]

Research and Development Team, Nano bio Research Center, Korea
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Polylactic acid (PLA) and polycaprolactone (PCL) are biomedical materials approved by the USA Food and Drug Administration (FDA) for their nontoxic and good biological compatibility. They are often used in tissue engineering or imitating extracellular matrix as functional materials for cell growth. PCL has excellent biological compatibility and toughness mainly applied in a controlled releasing carrier, such as drug loading, etc. However, PCL needs 2 - 4 years to degrade completely. PLA is the most used biodegradable material by far because it has good biological compatibility and significantly high strength and modulus. PLA's final products of degradation are CO2 and H2O, and the intermediate products are lactic acid and hydroxy acid, which are all accepted by the body. Although PLA's strength is high, there still exist problems such as low elongation, poor toughness and weak impact-resistance strength. Aiming at improving the slow degradation rate, poor hydrophilicity, weak strength and cell-attached force of PCL, introducing other biodegradable components to make up for the poor aspects of PCL performances has encouraged more research into materials such as PCL/PHBV, PCL/Collegen and PCL/Polyethylene glycol In this paper, biodegradable blending chips based on PCL and PLA were prepared using twin screw extruder. The PCL and PLA content varied in a ratio of 5/95, 10/90, 15/85 wt%. Scanning electron microscopy (SEM), differential scanning calorimetry (DSC), X-ray diffraction (XRD), differential scanning calorimetry(DSC) and biodegradability tests were used to investigate the structure, morphology and properties of PLA, PCL and PLA/PCL blending chips.

Poster Presentation : **MAT.P-545**

Material Chemistry

Event Hall THU 11:00~13:00

DEVELOPMENT OF HIGHLY POROUS MIXED METAL OXIDE UTILIZING LAYERED DOUBLE HYDROXIDE PRECURSOR AND EGG WHITE TEMPLATE Vidya Chandrabose , Jae - Min Oh

Chandrabose Vidya, **Jae-Min Oh**[1,*]

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ABSTRACT DEVELOPMENT OF HIGHLY POROUS MIXED METAL OXIDE UTILIZING LAYERED DOUBLE HYDROXIDE PRECURSOR AND EGG WHITE TEMPLATE Vidya Chandrabose , Jae - Min Oh Department of Energy and Materials Engineering, Dongguk University, Seoul, 04620, Republic of KoreaMixed metal oxide (MMO), which is regarded as one of the promising solid catalysts for various reactions, was prepared by calcining layered double hydroxides (LDH). In order to enhance specific surface area of MMO, egg white foam (EW) was utilized as porogenic template when LDH was precipitated. The LDH prepared with egg white form and the corresponding MMO was designated EWH and EWO, respectively. For comparison LDH and MMO without EW were prepared by coprecipitation and calcination. Several techniques such as X-ray diffraction, scanning electron microscopy, transmission electron microscopy and nitrogen adsorption-desorption isotherm was used for the characterization. LDH showed aggregated nanoparticle and EW specimens showed various random orientation platelet like morphology. The results confirmed that the pore volume of EWO (0.55 cm3/g) was more than twice of MMO (0.22 m2/g), showing the sacrificial role of EW in the development of pores during calcination. Specific surface area values of EWO were 247.79 m2/g; whereas that of MMO was 62.35 m2/g. The mean pore diameter of EWO was 8.92 nm, which was much smaller than that of MMO, 14.31 nm. It was concluded that the MMO with small pores and high specific surface area could be obtained with the help of sacrificial template of EW.

Poster Presentation : **MAT.P-546**

Material Chemistry

Event Hall THU 11:00~13:00

Development of ampoule material for improve scalp care by natural products

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Essential oil derived from natural products is widely used to antibiotic, antifungal, antimicrobial and aromatherapy. Moreover, due to the small molecular size and lipid solubility, it can be easily reach the layer of dermis through the skin epidermis. These properties are applicable to blending essential oils to increases the functional effect. We developed the new blending essential oils in various oils. In vitro evaluation was conducted by analyzing the antibacterial activity using skin bacteria and the inflammatory inhibitory effect using anti-inflammatory cell(raw 264.7). First, the clear zone size of skin bacteria was measured by the disc diffusion test, and then compared according to the essential oil mix ratio. Next, the anti-inflammatory effect was confirmed based on the cell viability. Five essential oil samples were obtained from two manufacturers. Cell viability of five essential oils was confirmed according to various concentrations, and three oils with the highest anti-inflammatory effect were selected. The three oils were also mixed in various ratios, and the ratio with the highest anti-inflammatory effect were selected. In conclusion, we optimized the essential oil combination to increase the effect of antibiotic, antifungal and antimicrobial in the skin.

Poster Presentation : **MAT.P-547**
Material Chemistry
Event Hall THU 11:00~13:00

Surface oxidation control of Fe-functionalized graphene oxide fiber for selective gas adsorption

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Porous carbon-based adsorbents suffer from weak binding energies with polar gas molecules. In order to promote selective adsorption functionality of carbon adsorbents, delicate surface oxidation control is needed. Herein, the oxidative surface of Fe-functionalized graphene oxide (Fe-GO) fiber is synthesized and controlled for selective VOCs adsorption. Through pH-induced reduction environment variation, the amount of transition metal (0.42~7.86%) and oxygen functional groups (30.54~38.73%) of Fe-GO fiber is successfully controlled. The difference in various physicochemical properties of the sample according to the pH of the solvent in which the fiber is made is investigated through an analysis device(FT-IR, XPS, BET, SEM, TEM, XRD). The adsorption capacity of the adsorbent is measured through GC's 6-port-valve system. The test result is fitted so that the ideal R-square value (0.97~0.998) is obtained using the Kinetics model most appropriate for the adsorption environment. As a result, Fe-GO fiber showed the highest adsorption amount (37.76~48.15mg/g) to Hexanone, Benzaldehyde, and Cyclohexanone and the lowest adsorption amount (0.14~0.63mg/g) to Hexane and C4-C5 Ketone. As a result, this sample show great potential in rapid and selective indoor air pollutant detection.

Poster Presentation : **MAT.P-548**
Material Chemistry
Event Hall THU 11:00~13:00

High Performance Separator for Li-S Battery Using Langmuir-Blodgett

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Lithium-sulfur (Li-S) batteries have been widely emphasized as an alternative to commercial lithium-ion (Li-ion) batteries not only for their higher theoretical capacity values but also for abundance of sulfur in nature and its safety. However, highly soluble sulfur in electrolytes produces insoluble reaction intermediates and induces shuttle effect limiting long cycle life of batteries. Separators, which can filter reaction intermediates have been studied to effectively suppress shuttle effect. For example, polymer-based separators have been coated with oxide[1] or carbon[2] for additional effects on filtration via pore or electrical attraction/repulsion. In particular, metal-organic frameworks (MOFs) as coating materials have advantages of porosity and electrical property which can be adjusted for desired filtrating property.

Herein, we synthesized a polypropylene (PP) separator coated with two types of MOFs (i.e. MOF-5 and IRMOF-3) using Langmuir-Blodgett (LB) technique for lithium-sulfur battery. Unlike atomic layer deposition (ALD) and chemical vapor deposition (CVD), LB technique is applicable to a polymer-based separator since it does not require heating process for a monolayer coating. A separator was uniformly formed (3.27 Å for R_a; roughness average) by deposition of five molecular monolayer films (total thickness was ~47.5 Å) using LB, while zinc acetate dihydrate and terephthalic acid were used as precursors for MOF-5 (2-aminoterephthalic acid for IRMOF-3 was used instead of terephthalic acid). To note, LB-coated MOF (both MOF-5 and IRMOF-3 showed similar level of filtration) separator showed comparable degree of filtration (compared by Li_2S_8 penetration amount via UV-Vis spectroscopy) to slurry-coated MOF despite of its thin thickness (c.a. 4000 times thinner than slurry-coated one). Moreover, batteries with IRMOF-3 LB coated separators exhibited 1.13 times higher cycle stability (after 100 cycles, 54.26% of the initial capacity was retained) compared to one with non-coated separator (after 100 cycles, 48.83% of the initial capacity was retained). This suggests that MOF coating contribute to filtration ability, and heteroatom (i.e. nitrogen in IRMOF-3) has an additional effect of electrical interaction. Consequently, we can improve the cycle stability of Li-S batteries by applying a MOF-coating to separators via LB which can further contribute to commercialization of Li-S batteries.

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Poster Presentation : **MAT.P-549**

Material Chemistry

Event Hall THU 11:00~13:00

Near-infrared/Visible Light Induced Spatio-temporal Electrical Switch via Independent Multi-states of Photoresponsive Nanocomposite

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Multi-stimuli responsive materials are advantageous in that they can enhance the targeted response or bypass undesired reactions. Light is one of the most attractive stimuli since it allows remote spatio-temporal control, and can be multiplexed by varying properties (e.g., wavelength, intensity, irradiation time, pulse/continuous wave, etc.) which leads to multi- photoresponsive materials. However, the operating wavelength for such photoresponsive systems generally includes ultraviolet (UV) range which limits its applications in biomedical systems. Herein, we investigate near-infrared (NIR)/visible (Vis) light-responsive nanocomposite, which is consisted of rare earth elements (e.g., Yb, Er) doped $NaYF_4$ nanoparticles (NPs) embedded in azobenzene-incorporated polydimethylsiloxane (AzoPDMS), silk fibroin, and silver nanowire layers. Photobending (PB) via AzoPDMS/silk fibroin bilayer is induced by 400–700 nm of Vis light, while upconversion photoluminescence (UCPL) via embedded NPs is activated by NIR light at 980 nm. The excitation wavelength of photoluminescence (PL) is successfully shifted from UV (λ = 365 nm) to NIR (λ = 980 nm) range via photon upconversion in rare earth elements doped on NPs. Independent operation of PB and UCPL enables multi-states of electrical stimulation and real-time location tracking. Dual photoresponsive nanocomposite film is successfully applied as a biological stimulator accompanied by a locational indicator which can give electrical pulse stimulation treatment, and further can be applied for non-invasive biomedical devices.

Poster Presentation : **MAT.P-550**
Material Chemistry
Event Hall THU 11:00~13:00

Reversible Nanoscale Molecular Communication System

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Nanoscale molecular communication (NMC) is a bio-inspired communication paradigm where information, in the form of molecules, is exchanged between nanomachines. This paradigm overcomes the limitations of traditional communication (using electromagnetic waves) in environments where execution was previously difficult such as confined spaces and aqueous media. Moreover, NMC provides greater efficiency, signal detection (sensitivity and selectivity), and biocompatibility compared to its traditional counterpart. Numerous theoretical models and computational simulations regarding NMC have been studied, however, a physical model has yet to be executed. Among various types of molecule transmission, flow-based molecular propagation mechanisms are prominent within the circulatory system which can be classified into laminar or turbulent flow based on Reynolds number (Re). Herein, physical models were constructed for comparing the NMC performance of two different flow mechanisms (laminar and turbulent) in real-time. Using each mechanism, the information carriers: sodium hydroxide (NaOH) and hydrochloric acid (HCl), were alternately propagated to citrate-stabilized gold nanoparticles (cit-AuNPs) receivers. The deprotonation and protonation responses of the receivers via base and acid addition, respectively, were monitored through zeta potential measurements. The reversibility and durability of the surface charge-switching response were evaluated and compared between the two systems. Our research provides experimentally executed flow-based NMC models (laminar and turbulent flow) capable of reversible signaling that can be monitored and stored in a real-time database. We anticipate our proof-of-concept to further expand the knowledge on NMC and allow for more intricate biological or bio-mimetic applications such as detecting and analyzing *in vivo* flow characteristics for vascular disease diagnoses where laminar and turbulent flow are commonly seen within healthy and atherosclerotic arteries, respectively.

Poster Presentation : **MAT.P-551**

Material Chemistry

Event Hall THU 11:00~13:00

Self-luminous C-14 incorporated Material with Core-shell Structure

Seoyoung Yoon, Dongjun Kim, Jiwon Kim*

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Nuclear energy technology such as alpha-/beta-voltaic nuclear battery has attracted increasing attention for its sustainable power supply regardless of the external environment. Since the performance of nuclear energy is highly dependent on the type of radioactive isotopes (e.g., radiation types, energy density and half-life), previous studies mainly focus on assessing the property of radioisotopes and optimizing its combination with various energy conversion materials. However, a structural design of radioisotope-energy conversion material pair has not yet been progressed much although its structure can significantly affect the energy conversion efficiency and safety. Herein, we have designed self-luminous ^{14}C incorporated material with core-shell structure by comprising $Ca^{14}CO_3$ as core and radioluminescent materials (e.g., ZnS:Cu) as shell. In this way, beta-radiation emitted from a radioactive source of ^{14}C is assumed to be fully delivered to radioluminescent shell, which not only enhances the radioluminescence efficiency but also prevents the radiation leakage. For the ease of experiment, $CaCO_3$ with similar chemical characteristics to $Ca^{14}CO_3$ was characterized along with UV-lamp. The shell thickness was controlled by varying the concentration of its precursors, which was confirmed by scanning electron microscopy (SEM) image and X-ray diffraction (XRD) pattern. Similarly, safe and durable self-glowing source can be fabricated if appropriately concentrated ^{14}C source is substituted. We believe a study on the structure design of ^{14}C-energy conversion material complex can provide new insights on application of ^{14}C which has been less dealt than other beta-sources (e.g., ^{3}H and ^{63}Ni) in limited fields (e.g., ^{14}C dating or labeling in biological field).

Poster Presentation : **MAT.P-552**
Material Chemistry
Event Hall THU 11:00~13:00

Core-shell MOF derived Porous Carbon with hierarchical pore structure and composition as Lithium-Sulfur Battery Cathodes

SeoYeah Oh, Seoyoung Yoon, Jiwon Kim*

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Lithium-sulfur (Li-S) batteries have been actively studied as one of the future energy storage devices for their high energy density (2500 Wh kg^{-1}), high theoretical specific capacities (1675 mAh g^{-1}) and abundance of sulfur in nature. However, developing cathodes of Li-S batteries is challenging owing to the insulating property, dissolution of lithiumpolysulfides (LiPS) and dramatic volume change of sulfur and LiPS during charge/discharge reaction. To minimize abovementioned issues, porous carbon with optimized structure and composition has been widely used as a cathode material. Herein, we synthesized a core-shell MOF-5-derived porous carbon whose pore structure and composition are hierarchically varied as a host material of sulfurs. Core-shell MOF-5 was synthesized by introducing functional group of $-NH^2$ into the shell of MOF-5 through a solvent-assisted ligand exchange method. By carbonization, nitrogen (N) was introduced from the outside to the inside of the porous carbon, and the pore structure changed hierarchically from micropore(exterior) to mesopore(interior). As a result, 2 ~ 5 at% of N was obtained in porous carbon and micropore/mesopore ratio increased compared to MOF-5. The heteroatoms outside the porous carbon structure chemically adsorbed LiPS, and micropores outside the porous carbon physically trapped LiPS, leading to an improvement of battery performance. Specifically, the performance of Li-S battery was enhanced in initial capacity (967 mAh g^{-1}) and showed cell cycle retention of ~75% even after 30 cycles compared to the pristine MOF-5. Therefore, we could achieve a high capacity and long-term cell cycle stability by optimizing the structure and composition of MOF-5 derived porous carbon. We believe that systematic study on both chemical and physical effects of core-shell structure can provide a direction for improving the limits of lithium-sulfur batteries.

Poster Presentation : **MAT.P-553**
Material Chemistry
Event Hall THU 11:00~13:00

Highly Stable Light-emitting Diodes based on Perovskite Quantum Dot/polymer Nanocomposites via Charge Transport Pathways on Dielectrics

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Perovskite quantum dots (PQDs) have become the most promising optoelectronic material in new generation displays and lighting devices due to their solution processability, narrow emission bands, and high quantum yield. PQDs are typically stabilized by long-chain aliphatic molecules such as oleic acid, oleylamine, or *n*-octylamine. However, these hydrocarbon chains are insulating and present a large potential barrier for charge transfer between PQDs in a solid film. Ligand exchange methods with smaller molecules have been studied to enhance charge transport, but there are limitations due to the low stability of PQDs in solution and film as well as the fundamental insulating property of the organic ligands. Herein, we report $CsPbBr_3$ QD/polymer nanocomposites of which charge transports through the charge transport pathway induced by the dielectric breakdown of the polymer (*e.g.*, polydimethylsiloxane, polystyrene, poly(2-vinylpyridine)). In the uniformly dispersed PQD/polymer nanocomposite, dielectric breakdown is induced by controlling the polymeric gap between PQDs to be wider than the charge tunneling distance limit (≤ 4.3 nm). The charge transport pathway formed only in polymer regions between adjacent PQDs was found to be mainly of nanoscale carbon filaments. Its energy level is expected to be similar to that of other carbon-based nanomaterials, which could improve charge injection and transport in the PQD film. In addition, the polymer matrix increases stability by preventing the penetration of oxygen and moisture, while it increases the quantum efficiency by preventing the formation of a pinhole which causes the leakage current. Our study suggests a next-generation design strategy for PQD-based LEDs, and further can be applied to optoelectronic devices such as photovoltaic devices and photodetectors.

Poster Presentation : **MAT.P-554**

Material Chemistry

Event Hall THU 11:00~13:00

Metal Hydroxide Nanoparticle Deposited Porous Carbon as Electrodes for High Performance Supercapacitor

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Increasing demand for diverse electronic equipment and vehicles has casted much attention on EESC (electrochemical energy storage and conversion) devices[1]. Among various EESC devices, pseudocapacitors, which mainly utilize transition metal oxides or hydroxides[2-3], have been one of the strong candidates for such applications as they provide high power density and cycle stability. However, transition metal hydroxides have limitations, such as low reactivity and electrical conductivity.

This study suggests growing transition metal hydroxide nanoparticles (THNPs; $Ni(OH)_2$, $Co(OH)_2$, $Ni_xCo_{1-x}(OH)_2$) inside the nitrogen-doped porous carbon through electrodeposition; the nitrogen-doped porous carbon can facilitate electrochemical reactions owing to high surface area, electrical conductivity, and wettability. The THNPs were uniformly deposited inside nitrogen-doped porous carbons by electrodeposition with variations in total charge of deposition and ratios of Ni^{2+} and Co^{2+} ions (Ni:Co = 1:0, 1:1, 0:1). THNPs could achieve higher capacitance than bulk transition metal hydroxides since intercalation and de-intercalation of electrons are facilitated by increased reaction sites. All of THNP-deposited NPCs showed high capacitance (> 2000 F/g), and $Ni_xCo_{1-x}(OH)_2$ NPs showed the highest capacitance (2706 F/g) possibly due to the synergistic effect from both ions. Systematic analysis of how the metal ion ratio and total charge affect the pseudocapacitors' performance can lead to further understanding of reaction mechanisms and applications in various future energy storage devices.

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Poster Presentation : **MAT.P-555**
Material Chemistry
Event Hall THU 11:00~13:00

Time-controlled nanoscale delivery system

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Delivering cargoes at desired time points and positions is inevitable for a time-dependent reaction involving multiple cargoes. However, several challenges (random walk motion of cargoes, interference between multiple cargoes, and driving forces with limitation in biological applications) hinder spatiotemporal control of cargo delivery in nanoscale, especially within a short time difference of less than a few minutes. Herein, we report a time-controlled active delivery system via multiple nanomotors moving at different velocities under the same magnetic field (i.e., constant and rotating magnetic field) and releasing cargoes at the desired position by temperature change upon irradiation. Nanomotors consist of nickel head, gold bridge, flexible silver filament, and gold tail encapsulated with poly (N-isopropylacrylamide) (pNIPAm) based hydrogel. Nickel and flexible silver segments rotate and induce the propulsion of nanomotors in response to the external rotating magnetic field, while the gold head converts near-infrared (NIR) light into heat by photothermal conversion causing the encapsulating thermal-responsive hydrogel to release loaded cargoes. Our nanoscale delivery system showed several tens of minutes of the arrival time difference, which can be varied by adjusting the applied magnetic field (e.g., frequency) and the length of each compartment within nanomotors. We believe our time-controlled delivery system composed of multiple nanomotors can be effective in time-dependent reactions requiring delivery of multiple cargoes within the active time frame (e.g., genetic manipulation via CRISPR*/Cas9 system, bone disease).

*Clustered Regularly Interspaced Short Palindromic Repeats/CRISPR-associated protein 9

Poster Presentation : **MAT.P-556**

Material Chemistry

Event Hall THU 11:00~13:00

Orientation Control of Lyotropic Chromonic Liquid Crystals in the Capillary Bridge

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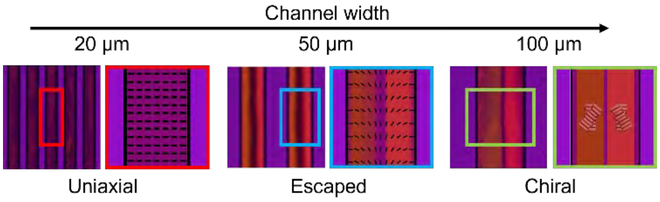
Well-ordered lyotropic chromonic liquid crystals (LCLCs) composed of 1D aggregates of disc-shaped molecules in water are widely used for display, sensor, and biotechnology. To apply LCLCs to potential applications, uniformly controlled structures in a large area are essential. Thus, various methods have been suggested, such as topographic confinement, mechanical shearing, and applying a magnetic field. Especially, many studies on micro-scale topographic confinement of LCLCs have been conducted. However, only one type of surface anchoring condition, planar or homeotropic anchoring, has been adopted to control the orientation of LCLCs in the previous studies. It means that the orientation of the LCLCs can be only globally controlled, but local confined structures might not be finely addressed. Here, we investigate the multi-dimensional orientation of the lyotropic chromonic liquid crystal (LCLC) in the capillary bridge surrounded by air walls made of glass and patterned silicon hybrid cells. The optical textures of uniaxial, escaped, and non-symmetric chiral LCLCs generated depending on the width of the capillary bridge are directly observed by polarized optical microscopy (POM), which are figured out using image analysis and simulations. Our platform can provide a new concept for orienting LCLC and can be applied to other systems using soft matters.



Poster Presentation : **MAT.P-557**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of PtAu Double-layered Nanoframes and their Enhanced Electrocatalytic Performance via Light Irradiation

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Nanoframe catalysts have attracted tremendous attention due to their intrinsic large surface area and tunable compositions. To date, many efforts have been made to achieve enhanced catalytic activity of nanoframe catalysts. However, these efforts are mainly focused on increasing their intrinsic catalytic activity. Herein, we synthesized complex PtAu double-layered nanoframes with intra-nanogap in a single nanostructure. By applying systematically designed chemical toolkits such as well-faceted overgrowth of Au, edge-selective deposition of Pt, and selective etching of inner Au, we could get PtAu double-layered nanoframes with intact two nanoframes in a single entity. By precisely controlling the experimental parameters such as counter halide ions (Cl^- and Br^-) and existence of Ag^+ ions, we figured out a successful route to synthesize double-layered nanoframes with structural robustness. Furthermore, due to increased surface area in a single nanostructure, electrocatalytic activity (i.e. methanol oxidation reaction) of PtAu double-layered nanoframes was increased compared to that of PtAu single-layered nanoframes. And with the aid of Au which is well-known as light-responsive metal, catalytic performance of PtAu double-layered nanoframes became higher. We expect this synthesis of PtAu double-layered nanoframes opens a new way to fabricate nanoframe structure with intra-nanogap and it is advantageous in terms of having higher surface area, which is important for catalyst.

Poster Presentation : **MAT.P-558**

Material Chemistry

Event Hall THU 11:00~13:00

Fabrication of Crystalline Silicon Nanowire Arrays using Deep Reactive Ion Etching Process

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Nanostructures have fascinating physical properties that the bulk material doesn’t exhibit. Especially, the optical and electrical properties of silicon nanowires (SiNWs) have attracted much attention for application in various devices such as solar cells and photodetectors. These characteristics can be systematically controlled by changing their physical dimensions (e.g., diameter and length). Consequently, it is the key to controlling the size of nanowires precisely to realize desired properties.This study demonstrates how to fabricate vertical nanowire arrays using electron beam lithography (EBL) and deep reactive ion etching (DRIE) process. The DRIE process, as one of the dry etching processes, is a highly anisotropic etching process. By providing high ion current density, it enables to etch silicon with fast etching rates and to produce nanostructures with a high aspect ratio compared to other dry etching processes. Therefore, it is a very suitable method for vertical SiNW arrays fabrication. Furthermore, this study focuses on the morphological changes of the SiNW arrays with various pitches and diameters by controlling temperature and the flow rate of SF_6 and C_4F_8 gases during the DRIE process.

Poster Presentation : **MAT.P-559**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and gas absorption of kraft lignin-poly(ethylene imine) (PEI) composite

Kyung-Hee Cho, Eun-Bum Cho*

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As environmental issues are emerging around the world, interest in the use of eco-friendly materials is increasing. Lignin, a biodegradable polymer abundant in nature, contains a benzene ring and an OH group and has good reactivity, so its use as an adsorbent is being considered. In fact, since the proportion of lignin used as an industrial material is insignificant, it is necessary to increase its practicality through proper mixing with other materials.In this experiment, poly(ethylene imine) (PEI), which is often used as an additive polymer for CO_2 adsorption, was crosslinked with lignin to investigate the effect on CO_2 adsorption. We used PEIs with different molecular weights, and hexamethylene diisocyanate (HMDI) and 4,4’-methylenebis(phenylene isocyanate) (MPI) as linkers between PEI and kraft lignin. The synthesized sample were analyzed with ^{1}H NMR, ^{13}C NMR, and FT-IR to confirm chemical bonds. In addition, thermal stability and CO_2 adsorption capacity were analyzed by TGA. This study was supported by the Human Resource Development Programs for Green Convergence Technology funded by the Korea Ministry of Environment(MOE).

Poster Presentation : **MAT.P-560**
Material Chemistry
Event Hall THU 11:00~13:00

Thiolated Amino Acids Based Synthesis of Tip-Modified Au Double Rings for SERS Measurement

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There are lots of tip-modified nanoparticles using for biosensor, catalyst, etc. Previous synthetic method of spiky structures was adding silver ions or using organic polymers. Thiol-containing amino acids can be also used for synthesizing tip-modified nanoparticles, especially Au spiky double rings (ASDRs). We successfully grow sharp tips on the Au double rings. It is possible to control the lengths of tips by tuning the concentration of amino acids or incubation time. We monitored the longer tips in the long wavelength of their localized surface plasmon resonance (LSPR) profiles. Precedent research showed that Au double rings enhanced surface-enhanced Raman scattering (SERS) intensity because of their intra-gap. Tips on the Au spiky double rings acted as a lightning rod, resulted in making hot spots. According to these results, tip-modified Au double rings can be used for an excellent substrate for SERS measurement.

Poster Presentation : **MAT.P-561**

Material Chemistry

Event Hall THU 11:00~13:00

Small-sized Deformable Shear Sensor Array for Direct Monitoring of Shear Force and Shear Distribution

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Artificial tactile sensors aim to mimic human tactile sensing by monitoring mechanical stimulus. They can be applied to a wide range of fields such as robots, healthcare devices, prosthetics, and wearable devices. An array of shear sensors is essential in tactile sensation as well as pressure sensors. Surprisingly, however, the shear sensor array has been rarely investigated mainly due to its structural complexity to measure the horizontal forces from various directions and also due to the mechanical softness required for preventing the slip of an object. Here, we fabricate an array of small shear sensors that can recognize both shear force and shear distribution. All the device components are made of deformable materials to acquire the softness of the sensor. This work presents a novel design for the small-sized shear sensor array and the required material conditions for the design. By using an ion gel as the capacitive sensing material, the shear sensor array shows high sensitivity and excellent reliability under repeated shear forces. This work demonstrates playing a computer game with the shear sensor and sensing the frictional force distribution, which is possible through the recognition of multiple shear stimuli and shear distribution when static/dynamic shear forces are simultaneously applied from various directions.

Poster Presentation : **MAT.P-562**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of aluminium doped nickel oxide nano-particles for electrochromic electrodes

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Doping with Aluminiuml cation is a very efficient way to modify the crystallinity and electronic properties of the Nickel oxde which could influence its electrochromic properties. In this study, we synthesized pure and Al doped NiO nanoparticles by co-precipitation method and chracterized by XRD, TGA, FE-SEM, EDS and UV-Visible spectrometer.The pure and Al doped NiO thin fims were coated on indium tin oxide(ITO)/PET substrates by wet coating technique. The electrochemical and electrochromic performance of the films were measured by cyclic voltammetry in 0.1M $LiClO_4$/PC electrolyte solution.

Poster Presentation : **MAT.P-563**
Material Chemistry
Event Hall THU 11:00~13:00

Effects of anion substitution on sulfide-aluminum based solid electrolyte for all-solid-state batteries

Jihun Roh, Seung-Tae Hong[1,*]

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[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

As increasing demands of electric vehicle (EV) and energy storage systems (ESS), lithium-ion all-solid-state batteries (ASSBs) have been attracted great attention due to their intrinsic safety and high energy density. In the perspective of mechanical properties and low-cost synthesis process, sulfide solid electrolytes (SEs) have been attracted for recent decades. Sulfide-based lithium ion conducting materials generally obtained through the substitution of immobile cations in the unit cell into iso- or aliovalent cations, results conducting ion vacancies or interstices in the unit cell or symmetry change in crystal structure. Herein, we report anion-substituted sulfide-aluminum based solid electrolytes (ASSAs) with enhanced ionic conductivity around two orders of magnitude from pristine crystal structure, owing to conducting ion vacancies or symmetry change in crystal structure. ASSAs were synthesized via solid-state reaction with high-energy ball milling. Crystal structures of ASSAs along the anion-substituted series were analyzed through powder X-ray diffraction data. Temperature-dependent Electrochemical impedance spectroscopy showed significantly decreased activation energy of ASSAs compared to pristine. To understand the stable conducting ion defect sites along the substitution series, DFT calculations were conducted to four Li-defect ASSA models, resulted reasonable Li-defect sites which in line with crystal structural data. ASSAs still face low ionic conductivity to be used as a SEs, however, this report suggests anion-substitution could be applied as an efficient strategy to improve ionic conductivity of crystal structure.

Poster Presentation : **MAT.P-564**

Material Chemistry

Event Hall THU 11:00~13:00

Superatom-in-Superatom $[RhH@Ag_{24}(SPhMe_{2})_{18}]^{2-}$ Nanocluster

Hanseok Yi, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Superatom is a cluster of atoms that mimic the properties of an element. Atom-precise metal nanoclusters with protecting ligands are also considered one of the superatomic complexes. In the nanocluster systems, heterometal doping is a powerful method for tunning the physicochemical properties of homometallic nanoclusters. While the heterometals doped into such nanoclusters predominantly include transition metals with closed d-shells, the doping of open d-shell metals remains largely unexplored. Recently, we reported the first synthesis of a $[RhH@Ag_{24}(SPhMe_{2})_{18}]^{2-}$ nanocluster, in which a Rh atom with open d-shells ($[Kr]4d^{8}5s^{1}$) is incorporated into the Ag_{24} framework by forming a RhH entity. Combined experimental and theoretical investigations showed that the RhH dopant was a superatomic construct of a Pd atom ($[Kr]4d^{10}$). Additional studies confirmed that the $[RhH@Ag_{24}(SPhMe_{2})_{18}]^{2-}$ nanocluster was isoelectronic to the $[Pd@Ag_{24}(SPhMe_{2})_{18}]^{2-}$ nanocluster with the superatomic 8-electron configuration ($1S^{2}1P^{6}$). We demonstrated for the first time that a superatom could be incorporated into a cluster superatom to generate a stable superatom-in-superatom nanocluster.

Poster Presentation : **MAT.P-565**
Material Chemistry
Event Hall THU 11:00~13:00

A Study of Optimized Release Conditions for Development of Contact Lenses with a Drug

Seung Hyuck Bang[*], Sung Hwa Oh, Yuseon Noh

Jeonnam Bioindustry Foundation Nanobio Research Center, Korea

Objective: Nowadays, as the senior increases and the use of IT devices, the number of patients with dry eye syndrome due to damage to the tear layer is rapidly increasing, which is a major cause of significantly lowering the quality of life by lowering functional vision. Dry eye syndrome is very difficult to treat fundamentally, and it can cause secondary eye diseases such as keratitis due to corneal damage by inducing an immune response.Methods : Type 1 drug delivery system was made by synthesizing an amine group with hyaluronic acid having an aldehyde group. Type 2 was made a pH-sensitive nanoparticle drug delivery system containing drug. Contact lenses was evaluated the release of drug with varioous conditions using HPLC.Results : Dissolution amounts of both Type 1 and 2 was showed about 70% and 55% from total them after 12 hours and about 90% and 80% after 24 hours at pH 7.4 condition, respectively. After changing condition with pH 5.5, we evaluated the dissolution amounts in the same way (pH 7.4). Dissolution amounts of both Type 1 and 2 was showed about 23% and 56% from total them after 12 hours and under 30% and 80% 24 hours, respectively. Lastly, it was confirmed that no dissolution amounts for 24 hours at the 4℃. Conclusion: It was confirmed that Type 1 was more sensitive to drug release according to pH than Type 2. It was confirmed that it can be used as drug-releasing contact lenses in the future.

Poster Presentation : **MAT.P-566**

Material Chemistry

Event Hall THU 11:00~13:00

Adsorptive removal of benzonitrile and carbazole from model green-diesel derived from microalgae using metal-organic frameworks with protonated amines

Gyudong Lee, Sung Hwa Jhung[1,*]

Chemistry, Kyungpook National University, Korea

[1]*Department of Chemistry, Kyungpook National University, Korea*

The effective utilization of microalgae-derived fuel is very important for our sustainability. Here, adsorptive denitrogenation of model green-diesel (with considerable nitrogen-containing compounds, NCCs) was investigated to check the feasibility of adsorptive purification of fuel, derived from microalgae that is composed of NCCs. A highly porous MIL-101(Cr) (named M101) metal-organic framework was firstly modified to introduce protonated amino groups on both the linker and metallic sites of the MOF. The functionalized MOFs including P-M101-NH_2-ED (P and ED mean ‘protonated’ and ethylenediamine, respectively), M101-NH_2-ED, and M101-NH_2 were applied (together with pristine M101 and a conventional activated carbon) in the adsorptive removal of N-containing compounds like benzonitrile (BENZ) and carbazole (CARB) from model green-diesel. The prepared P-M101-NH_2-ED showed the most effective performances in the adsorption, compared with any other adsorbents known thus far. For instance, P-M101-NH_2-ED adsorbed 15.6 and 3.6 times of BENZ and CARB, respectively, that of the activated carbon. The observed remarkable performances of P-M101-NH_2-ED (Q_0 values for BENZ and CARB are 500 and 455 mg/g, respectively), although with lower porosity than other M101s, for BENZ and CARB adsorption could be explained mainly with hydrogen bonding and hydrogen bonding/cation-π interactions, respectively. Moreover, P-M101-NH_2-ED was recyclable in several cycles after simple ethanol washing. Therefore, P-M101-NH_2-ED could be suggested as a plausible adsorbent to remove NCCs from green-diesel, based on remarkable performances and facile reusability.

Poster Presentation : **MAT.P-567**

Material Chemistry

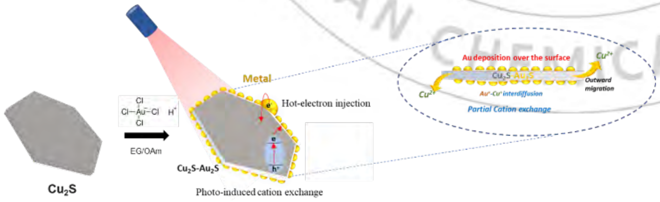
Event Hall THU 11:00~13:00

Designing 2D hollow nanoreactors of Cu_2S-Au through cationic exchange for efficient plasmonic catalysis

<u>Sampathkumar Jeevanandham</u>, In Su Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea

Control over the nanostructured heterointerface evolution with well-defined structural order, particle size and junction geometry offer high tunability in their physicochemical properties. However, designing such rational morphologies in metal-semiconductor hybrids with distinct shape/composition-dependent features still remains a synthetic bottleneck. Herein, a facile ligand controlled photochemical cation exchange process has been utilized as post-synthetic modification strategy to synthesize 2D hollow Cu_2S-Au nanosheets with tailorable optical properties. The interfacial electron transfer from the excited Cu_2S to Au surface in the heteronanojunctions and the mechanism of interdiffusion to form 2D hollow Cu_2S-Au_2S intermediate nanostructures is expected to decipher the effect of plasmon enhanced absorption and emission in photocatalytic chemical reactions.



Poster Presentation : **MAT.P-568**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of Mesoporous Silica and Characterization of CO2 Adsorption through Room Temperature Reaction

Jong-tak Lee, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

Many researches are being conducted using MOFs, zeolites and porous silicas for CO2 adsorption studies. Among them, in the case of porous silica, many studies have been conducted due to the advantages of thermal stability and functional group introduction. In this study, the calcination treatment for porous silica production and extraction and removal methods at room temperature were compared. The physical properties of the synthesized material were analyzed using XRD, TEM, N2-sorption and TGA, and the CO2 adsorption performance was analyzed after introducing an amine functional group. As a result of N2-sorption measurement, it was confirmed that the specific surface area of the two materials was similar, but there was a large difference in the pore volume. In the case of silica synthesized through extraction and removal at room temperature, a larger pore volume was measured, and it was confirmed that the CO2 adsorption performance was significantly improved due to an increase in the introduction of an amine functional group.

Poster Presentation : **MAT.P-569**

Material Chemistry

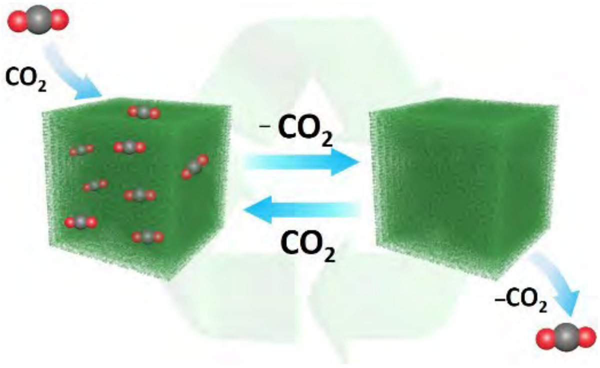
Event Hall THU 11:00~13:00

Hierarchical metal-organic aerogel as a highly selective and sustainable CO_2 adsorbent

Heehyeon Lee, Youngtak Oh[*], Seok Min Yoon[1,*]

Center for Environment,Health and Welfare Research, Korea Institute of Science and Technology, Korea
[1]*Department of Chemistry, Wonkwang University, Korea*

Typical amorphous aerogels pose great potential for CO_2 adsorbents with high surface area and facile diffusion, but they lack well-defined porosity and specific selectivity inhibiting utilization of their full functionality. To assign well-defined porous structures to the aerogel, hierarchical metal-organic aerogel (HMOA) is designed, which is consisted of well-defined micropores (d ~ 1 nm) by coordinative integration with chromium(III) and organic ligands. Due to the hierarchical porous networks with intrinsically flexible coordination in aerogel, the HMOA has excellent porous features of high surface area and a reusable surface with appropriate binding energy for CO_2 adsorption. The HMOA features high CO_2 adsorption capacity, high CO_2/N_2 IAST selectivity, and vacuum-induced surface regenerability (100% through 20 cycles). Further, the HMOA could be prepared via simple ambient drying methods while retaining the microporous network, although the simple drying process collapsed most gels' porosity. This unique surface-tension-resistant micropore formation and flexible coordination systems of HMOA pose great potential for a CO_2 adsorbent with industrial scalability and reproducibility.



Poster Presentation : **MAT.P-570**

Material Chemistry

Event Hall THU 11:00~13:00

Application of functionalized mesoporous silica films for exosome separation

Guanghai Piao, Ji Man Kim[1,*]

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[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Exosomes are cup-shaped lipid bilayer vesicles, ranging in size from 30-150 nm, which are secreted into body fluids by various cells in living organisms in the form of cytosol, and belong to one of the extracellular vesicles. As the research progresses, exosomes are used in a wide range of applications, such as early cancer markers and targeted drug carriers. How to isolate exosomes from body fluids rapidly and non-destructively is the difficulty faced at present. Traditional ultracentrifugation, polymer precipitation, and microfluidic techniques have various drawbacks. To achieve high throughput, high recovery, and non-destructive separation of exosomes, using the advantages of mesoporous silica with controllable pore size, pore length, and orientation. Mesoporous silica films with vertical pore channels were designed. The functionalized Mesoporous Silica Film (FMSF) was synthesized by a simple functionalization of the film to achieve reusability, while the exosomes in complex body fluid samples were rapidly separated by a size exclusion method.

Poster Presentation : **MAT.P-571**

Material Chemistry

Event Hall THU 11:00~13:00

Improving Lithium-Sulfur Battery Performances by Using Conjugative Porous Polymer as the Sulfur Support: the Case of N-containing Porous Aromatic Framework 41

Qian Wang, Ji Man Kim[1,*]

Department of Chemistry, Sungkyunkwan University, China

[1]*Department of Chemistry, Sungkyunkwan University, Korea*

N-containing porous aromatic framework 41 (PAF-41) with hierarchical porous structure has been readily synthesized through $AlCl_3$ catalysed Scholl reaction by using triphenylamine as the monomer. The extended skeleton of PAF-41 is constructed by N-bridged biphenyl groups to generate a consecutive conjugative electronic structure. The hierarchical porous skeleton and the presence of N atoms effectively confine the electroactive species by synergistic physisorption and chemisorption to alleviate the shuttle effect that is induced by the soluble polysulfides. These features render the sulfur impregnated PAF-41 (SPAF-41) improved lithium sulfur battery performances, especially the cycling stability. SPAF-41 composite cathode with high sulfur loading of 72 wt% exhibits enhanced rate capability and excellent cycling performance. The cell delivers a high capacity of 725.8 mAh g^{-1} at 0.5 C in the first cycle and sustains a reversible capacity of 491.4 mAh g^{-1} after 500 charge-discharge cycles. A low decay rate 0.06% per cycle is achieved. The well conductive PAF-41 support bestows the cell high Coulombic efficiency of 97.36%.

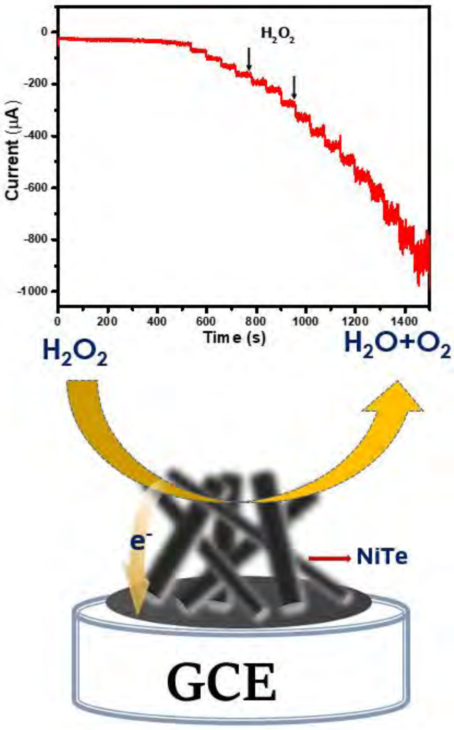
Poster Presentation : **MAT.P-572**
Material Chemistry
Event Hall THU 11:00~13:00

Facile Synthesis of Nickel Telluride electrocatalyst for an effective detection of Hydrogen Peroxide

Loganathan Kulandaivel, Hyun Jung*

Department of Chemistry, Dongguk University, Korea

Recently, the development of highly efficient electrocatalyst with an excellent stability in the electrochemical detection of analyte is an important research topic of biosensors. Herein we designed a hierarchical NiTe rod like nanostructure via one-pot hydrothermal technique. The structural and morphological properties of the resultant material were explored using X-ray diffraction spectrum (XRD), FT-IR, Raman, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray analysis (EDX), and X-ray photoelectron spectroscopy techniques. These analyzes confirmed the formation of NiTe nanorods (NR) with required stoichiometry. The electrochemical sensing properties of the NiTe were performed by the fabricated NiTe-NR modified GCE using Cyclic Voltammetry (CV) and amperometric (i-t) techniques. The results suggest the effective response of NiTe-NR/GCE with a low limit of detection (LOD) and considerable sensitivity in the detection of H_2O_2. Moreover, the selectivity data exhibited excellent anti-interference property of NiTe-NR/GCE electrode towards H_2O_2 in the presence of possible interfering agents viz. uric acid, ascorbic acid, dopamine, glucose, and melamine.


H_2O_2
0
-200
-400
-600
-800
-1000
Current (μA)
0
200
400
600
800
1000
1200
1400
Time (s)
H_2O_2
H_2O+O_2
e^-
NiTe
GCE

Poster Presentation : **MAT.P-573**

Material Chemistry

Event Hall THU 11:00~13:00

Ultrafine cobalt nanoparticles decorated mesoporous graphene as an electrochemical sensor for hydrogen peroxide detection

JeongWon Park, C. Justin Raj, Periyasamy Sivakumar, Hyun Jung*

Department of Chemistry, Dongguk University, Korea

Transition metal nanoparticles are considered as a candidate for replacing precious noble metallic catalysts due to their high surface-to-volume ratios and large number of active sites. However, agglomeration of nanoparticles during the synthesis process lowers their specific surface area and which leads to a significant reduction in their catalytic activity. To overcome this problem, the in-situ growth of metal nanoparticles on carbon-based support is a promising solution. Herein we report the fabrication of cobalt nanoparticles decorated mesoporous graphene (MGCo) with an interpenetrating porous network by hydrothermal process utilizing graphene oxide (GO) and self-assembled triblock copolymer template (Pluronic P123) in the presence of cobalt chloride. The structural, morphological and, chemical compositions of the obtained MGCo were characterized. And the fabricated MGCo has high BET specific surface area (~ 609.9 m^2 g^{-1}) with three-dimensional interconnected network. Besides, the high-resolution TEM image and energy dispersive X-ray spectrum reveals that the obtained MGCo has decorated with spherical cobalt metal (Co) nanoparticles with oxidized outer layer (CoO) of size ranges from 6~8 nm. Further, the modified glassy carbon electrode for hydrogen peroxide sensor was fabricated using MGCo and their preliminary performances were evaluated and discussed in detail.

Poster Presentation : **MAT.P-574**
Material Chemistry
Event Hall THU 11:00~13:00

High thermoelectric performance of p-type SnSe via introducing Y and vacancy to the crystal lattice

Hyungseok Lee, Chung In*

Center for Correlated Electron Systems (IBS) and School of Chemical and Biological Engineering, Seoul National University, Korea

SnSe single crystals shows extraordinarily high thermoelectric (TE) figure of merit figure of merit, ZT, of ~2.6 at 923 K along *b*-axis mainly due to its highly favorable, intrinsic electronic and phonon structures. However, single crystal form is subject to poor mechanical stability, and its preparation requires elongated processing time and high cost. This requests the development of polycrystalline counterparts with similar or even higher performance for broad-based commercialization of this emerging technology. To achieve this goal, it is important to discover effective alloying/dopant agents and optimal compositions. In this presentation, we discuss high thermoelectric performance of hole-doped polycrystalline SnSe samples by the dual incorporation of Y and vacancy. Despite inducing favorable electronic band structure, Y doping to the SnSe crystal lattice has been considered to deteriorate electrical transport properties of SnSe because of the common trivalent oxidation state of Y with Se atom. In this work, we intentionally introduce cationic vacancy serving as hole donor in the SnSe lattice, consequently compensating the loss of carrier concentration by Y doping. The resulting point defect and vacancy simultaneously scatter heat-carrying phonon, thereby lowering lattice thermal conductivity. All these induced effects synergistically improves power factor to ~5.8 μW cm^{-1} K^{-2} and decreases lattice thermal conductivity to ~0.17 W m^{-1} K^{-1}, giving a high peak ZT of ~1.7 at 800 K.

Poster Presentation : **MAT.P-575**

Material Chemistry

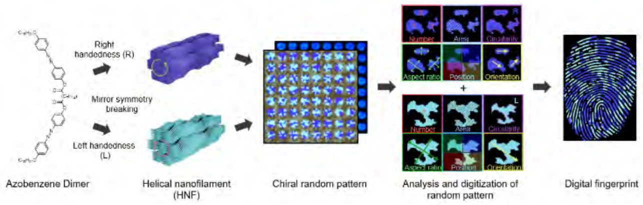
Event Hall THU 11:00~13:00

Physical unclonable anti-counterfeiting labels enabled by spontaneous mirror symmetry breaking

Hyewon Park, Dong Ki Yoon*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Advances in smart technologies continue to change the world and enhance the quality of our lives. At the same time, however, the demand for developing security systems to combat counterfeiting has been increased. In this regard, hardware-based physical unclonable function (PUF) has recently been in the spotlight as an effective alternative. It is a device that provides a unique digital fingerprint by utilizing the inherent randomness generated during the manufacturing process. Among various types of PUFs, promising novel approaches using optical signals generated from nanoparticles, fluorescent materials, and biomaterials have been proposed. Despite their high performance, they have some drawbacks, which limit their practical applications. Therefore, for real-world applications, there is a need to develop an advanced optical PUF that can be easily fabricated while ensuring security performance. In this study, we present a novel optical PUF based on spontaneous mirror symmetry breaking of molecular self-assembly using an achiral bent-shaped azobenzene dimer with liquid crystalline properties. The molecules are spontaneously self-assembled to helical superstructure after phase transition, known as helical nanofilament (HNF). Moreover, HNF can be aligned according to UV irradiation to form photonic crystal. The chiroptical signals from each chiral domain are digitized for authentication through image processing. The statistical analyses demonstrate that our chiral PUF has high encoding capacity, recognition rate, and reconfigurability, as well as a high level of robustness. Our strategy of incorporating natural randomness into artificial devices is expected to be a potential candidate for next-generation security systems.



Poster Presentation : **MAT.P-576**

Material Chemistry

Event Hall THU 11:00~13:00

Naphthalene-diimide-based small molecule containing a thienothiophene linker for n-type organic field-effect transistors

Gyeong Seok Lee, Yun Hi Kim[1,*]

Chemistry, Gyeongsang National University, Korea

[1]*Department of Chemistry, Gyeongsang National University, Korea*

A naphthalene diimide (NDI)-based small molecule with a thienothiophene linker donor unit (NDI-TT-NDI) was newly synthesized for the purpose of serving as the active material of solution-processable n-type organic field-effect transistors (OFETs). The thienothiophene linker was introduced to the donor site between the two NDIs to impart planarity to the molecular backbone, which is favorable for inducing high crystallinity, and the morphological and crystal characteristics of the resulting film were analyzed. We also investigated the effect of the additional annealing treatment applied to the NDT-TT-NDI films changed their orientation such that the molecular ordering and crystallinity of the film were significantly improved at a specific annealing temperature. The optimally annealed NDI-TT-NDI film exhibited a distinct edge-on molecular orientation with a narrow intermolecular π-π stacking distance, which is advantageous for lateral charge transport along the stacks. Consequently, an optimally annealed NDI-TT-NDI-based OFET exhibited electron mobilities of up to 0.032 $cm^2 V^{-1} s^{-1}$ and an on/off ratio of 1.0×10^7

Poster Presentation : **MAT.P-577**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and characterization of tungsten carbide nanoparticles stabilized in mesoporous three-dimensional (3D) graphene

JeongWon Park, Periyasamy Sivakumar, C. Justin Raj, Hyun Jung*

Department of Chemistry, Dongguk University, Korea

Due to depletion of fossil fuel and environmental pollution, utilization of hydrogen energy is one of the promising alternative energy sources since it produces clean product with high energy density. Therefore, hydrogen evolution reaction (HER) through water electrolysis draws attention as the important technology in the large-scale production of hydrogen fuel. Noble metals represented by platinum (Pt) is highly active for HER, nevertheless, it suffers for commercial usage because of its high cost and scarcity. Recently, tungsten carbide (WC) is considered as a possible replacement of Pt, but the synthesis procedures are often complex or demand high energy consumption. In this report, tungsten carbide nanoparticles incorporated in mesoporous graphene (MGWC) were fabricated by carburization process using simple mixture of tungstate solution and mesoporous graphene (MG). The obtained MGWCs were characterized by X-ray diffraction, scanning electron microscopy, and N_2 adsorption-desorption measurements, respectively. The morphological analysis reveals that the porous character of MG is still preserved even after carburization process. In addition, the electrocatalytic measurements were performed for the sample to validate the electrochemical HER activity. And the optimized sample exhibited an overpotential of -170 mV (Vs. RHE) at a benchmark current density of $j = 10\ mA/cm^2$ (η_{10}), which comparable or even higher than other related samples.

Poster Presentation : **MAT.P-578**

Material Chemistry

Event Hall THU 11:00~13:00

Ce-MOFs derived CeO_2-MnO_2 catalysts for CO oxidation

Lianghao Song, Ji Man Kim[1,*]

Department of Chemistry, Sungkyunkwan University, China

[1]*Department of Chemistry, Sungkyunkwan University, Korea*

CeO_2-based catalysts are widely studied in the catalysis fields. Developing one novel synthetic approach to increase the intimate contact between CeO_2 and secondary species is of particular importance for enhancing catalytic activities. Herein, we design an interfacial reaction between MOF-derived Carbon and $KMnO_4$ to synthesize CeO_2-MnO_2, where the Carbon is derived from the pyrolysis of Ce-MOFs under inert atmosphere. The MOF-derived Carbon is found to restrain the growth of CeO_2 crystallites at high calcination temperature, and more importantly, the intimate contact within CeO_2/C is conveyed to CeO_2/MnO_2 after interfacial reaction, which are responsible for high catalytic activity of CeO_2-MnO_2 towards CO oxidation.

Poster Presentation : **MAT.P-579**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis, crystal structures, optical and dielectric properties of complex perovskite oxynitrides $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ (M = Nb, Ta)

YangHun Kim, Young-il Kim[1,*]

Department of Chemistry, Yeungnam university, Korea
[1]*Department of Chemistry, Yeungnam University, Korea*

Oxynitride type complex perovskites $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ (M = Nb, Ta) were newly synthesized by the solid state reaction between Al_2O_3 and $Sr_5M_4O_{15}$ in the ammonia atmosphere. The formation of $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ is enabled by the concomitant Al^{3+} intercalation into the layered oxide $Sr_5M_4O_{15}$ along with the charge compensation from aliovalent O^{2-}/N^{3-} substitution. Rietveld analysis of synchrotron X-ray diffraction patterns indicated that both compounds adopt the body-centered tetragonal symmetry. As resulted from the nitride introduction, the band gaps of $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ are much narrower, compared with the respective $Sr_5M_4O_{15}$. Dielectric properties of $SrAl_{0.2}M_{0.8}O_{2.4}N_{0.6}$ are under study using the compacted pellet specimens.

Poster Presentation : **MAT.P-580**
Material Chemistry
Event Hall THU 11:00~13:00

Crystalline silicon microwire solar cells with light-scattering silica beads

Youri Lee, Kangmin Lee, Kwanyong Seo*

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea

Light absorption is one of the most important factors affecting the power conversion efficiency (PCE) of solar cells. However, since the position of the sun changes depending on the season and time, the light absorption of the solar cell is not constant. This is because the amount of light absorbed by the solar cell decreases as the angle of incidence of light reaching the solar cell increases. Therefore, it is necessary to minimize light absorption loss due to a change in the angle of incidence of light reaching the solar cell for maximizing solar power generation. In this study, we used microwire structures for maximizing light absorption and minimizing light absorption loss according to the angle of incidence of light. As a result, we confirmed that the PCE of the solar cell without the structure decreased by over 55% when the incident angle of the light changed from 0 to 60°, whereas the PCE of the solar cells with microwire structures decreased by less than 35%. Furthermore, we added the light-scattering silica beads, which is almost no self-light absorption, between the microwire structures to minimize light absorption loss according to the angle of incidence of light. This work provides a novel strategy to reduce the angular dependence of PCE degradation of the solar cells.

Poster Presentation : **MAT.P-581**

Material Chemistry

Event Hall THU 11:00~13:00

Ordered mesoporous Manganese Nickel Oxide was synthesized and characterized to improve the passability of current.

Chenglin Cui, Yelim Kwon[1], Hansol Kim[2], Ji Man Kim[1,*]

Department of Chemistry, Sungkyunkwan University, China
[1]*Department of Chemistry, Sungkyunkwan University, Korea*
[2]*Chemistry, Sungkyunkwan University, Korea*

Research on secondary batteries is becoming more active, and they play a very important role in modern life. Among them, the aqueous zinc ion secondary battery has received the most attention due to its low cost, low oxidation/reduction potential, excellent stability, abundant resources and large capacity. Despite these advantages of Zn anodes, finding suitable cathode materials for Zn-ion batteries is still a great challenge.In this study, we have successful synthesized ordered mesoporous Manganese Nickel Oxide(NMO) with three-dimensional cubic structure, high surface area and crystalline frameworks. It is synthesized by using a nanostructure replication method from a mesoporous silica template of KIT-6 and employed as electrode in aqua zinc-ion battery. Mn has a high capacitance in the cathode material. However, in the process of electrochemical reaction, Mn will dissolve and phase transition will occur immediately. Therefore, in order to inhibit Mn dissolution and phase transformation, different proportions of Ni were added to study the reaction. Ordered mesoporous NMO would have good electrochemical performances.

Poster Presentation : **MAT.P-582**

Material Chemistry

Event Hall THU 11:00~13:00

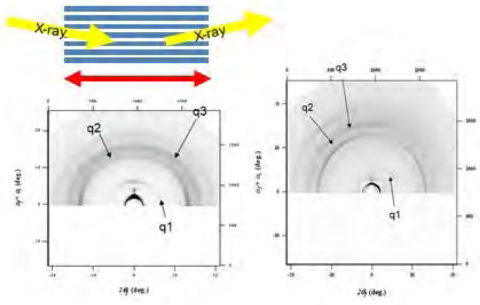
Circularly Polarized Light-sensing Photodetectors via Highly Oriented Liquid Crystalline Semiconductors

Yeong Seo Park, Hee Seong Yun[1], Dong Ki Yoon[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Chiral photonics has grown in importance for future optoelectronics, such as photon-based spin information transfer and quantum-based optical computing for data processing and encryption, using optoelectronic waves from stereoisomeric compounds. Due to the ongoing investigation of chiral photonics, developing devices capable of converting optical power into electrical signals still remains challenging. Previous research has required complex individual layers to distinguish chiral optical signals and to convert them into electrical currents separately or has suffered from reduced charge transport performance accompanied with poorly ordered molecular orientation. Herein, a [1]benzothieno[3,2-b][1]- benzothiophene (BTBT) derivative equipped with chiral alkyl pendant, a liquid crystalline semiconducting material, was designed and synthesized, thereby, allowing the facile fabrication of defect-free and highly oriented semiconductors in large areas. We believe that this novel material is thus a key for designing highly responsive circularly polarized light-sensing photodetectors, opening up the potential of organic semiconductors in chiral photonics.



Poster Presentation : **MAT.P-583**

Material Chemistry

Event Hall THU 11:00~13:00

Low-voltage Extended-Gate Thin-Film Transistor based Biosensor for Detecting Tau Protein

Ga Young Won, Young-Geun Ha[1,*]

Chemistry Department, Kyonggi University, Korea
[1]*Department of Chemistry, Kyonggi University, Korea*

Conventional diagnosis methods for Alzheimer disease (AD) have the advantage of providing high precision and selectivity, but have the disadvantage of taking a long time and expensive. To overcome for these limitations, this study fabricated a biosensor for early diagnosis of AD using TFTs that have the advantages of fast detection, inexpensive, and low voltage operating. At this time, an extended gate used as a sensing layer was applied to prevent damage to the transistor while directly contacting the electrolyte. First, this TFT is operated at a low voltage using a high-k ZrOx, as a gate dielectric, and the semiconductor uses indium gallium zinc oxide (IGZO). Heavily n^{++} doped Si wafer was used as the extended-gate and connected to the TFT. In order to check whether the EG-TFT manufactured in this way works well as a sensor, we first performed the most basic pH sensor using APTES. Then, the extended gate of TFT assembled cognitive function groups using APTES, glutaraldehyde, tau-aptamer to complete an biosensor, and this EG-TFT biosensor was able to successfully detect Tau of various concentrations.

Poster Presentation : **MAT.P-584**

Material Chemistry

Event Hall THU 11:00~13:00

An Exciplex host for Solution-Processed Green Phosphorescent Organic Light-Emitting Diodes

Bonju Koo, Hyejin Na, Jaemin Lee*

Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea

In recently years, solution-processing of organic light-emitting diodes is generally used in display industry due to its merits for using low materials, direct patterning, and low cost. However, solution-processing has disadvantages such as device’s low efficiency compared to vacuum evaporation. To solve this problem, the exciplex system applies the emission layer of OLEDs, which can be improving device’s efficiency and roll-off effect. The exciplex system is formed by mixing p-type materials and n-type materials, the difference between HOMO of p-type and LUMO of n-type must reach a certain level. For this purpose, it is necessary to synthesize a new materials that have low LUMO level or high HOMO level.In this work, a new n-type material has been synthesized and the optical properties of material have also been analyzed. We found out through the TRPL graph that excipelx is formed, and then a mixture of new n-type material and existing p-type material has been used for host of emission layer. Compared of single host or other n-type material, the results of OLED device with exciplex host have been seen high EQE, long lifetime and improving roll-off.

Poster Presentation : **MAT.P-585**

Material Chemistry

Event Hall THU 11:00~13:00

Bicontinuous Nanoporous Membrane Supported Metal Nanocatalysts: A New Type of Nano-reactors For Selective Partial Hydrogenation of Alkynes Under Continuous Flow Conditions

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[1]*School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea*

The bicontinuous nanoporous covalent frameworks are promising for immobilizing metal nanoparticles (MNPs). The frameworks have three-dimensionally continuous porous channel within the average pore diameter of 5~30 nm. Small sized MNPs are dispersed homogeneously into bicontinuous nanopore by wet impregnation method. By controlling the concentration of metal precursor solution, the size and(or) amounts of MNPs are adjusted precisely. The resulting nanoporous frameworks supported MNPs are used as catalytic nanoreactor in selective partial hydrogenation reaction of alkynes under continuous flow conditions. Because continuous flow systems maintain the initial reactant conditions, the catalytic nanoreactors demonstrated significant increase in selectivity on desired alkene product in comparison with conventional batch reactor. Moreover, high catalytic performance was obtained by adjusting various experimental parameters of continuous flow system (pressure, flow rate, and residence time).

Poster Presentation : **MAT.P-586**

Material Chemistry

Event Hall THU 11:00~13:00

Enhanced thermoelectric properties of AgPbBiS3 via halogen doping

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A member of sulfosalt minerals, AgPbBiS3 , appears to be promising for thermoelectric applications due to its high symmetry of cubic structure, complex chemical composition, and low electronic band gap. Nevertheless, pure synthesis and thermoelectric properties of AgPbBiS3 have not been well established. In this work, we present the synthesis of pure phase of halogen doped AgPbBiS3 by high-temperature solid-state reaction as well as its structural chemistry, thermal analyses and thermoelectric transport properties including electrical conductivity, Seebeck coefficient, and thermal conductivity. AgPbBiS3 is an n-type semiconductor with a band gap at 0.74 eV. It crystallizes in the NaCl type structure, where Ag, Pb, and Bi atoms are distributed randomly in the cationic site and S and halogen atoms are spread at the anionic site. Such a structural characteristic exhibits low thermal conductivity of ~0.7W/mK. The spark plasma-sintered dense pellet of AgPbBiS2.97Cl0.03 exhibits a maximum thermoelectric figure of merit (ZT) of ~0.4 at 823K.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-587**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and Characterization of New benzodithiophene fused electron acceptors For Organic Solar Cell

Yun Hi Kim*, Ji Eun Lee

Department of Chemistry, Gyeongsang National University, Korea

We synthesized and designed electron acceptors based on 6,6,12,12-tetrakis (3-hexylphenyl)-indacenobis (benzodithiophene) named ETBDTIC and ESTBDTIC, respectively. ESTBDTIC showed more red-shift absorption and deeper the lowest unoccupied molecular orbital(LUMO) and the highest occupied molecular orbital(HOMO) levels than ETBDTIC. Fill factor(FF) and short-circuit current density(Jsc) of ESTBDTIC based device were much higher than the FF and Jsc of ETBDTIC, while the ESTBDTIC showed lower open-circuit voltage(Voc) because it has thioalkyl group so that LUMO level becomes deeper. The ESTBDTIC-based device exhibited power conversion efficiency (PCE) of 7.78% with a Jsc of 13.92 mA/cm2, Voc of 0.92 V and FF of 60.50%; the corresponding values of ETBDTIC-based device were 5.11%, 11.24 mA/cm2, 0.96 V, and 47.30%. The charge transport, electronic properties, film morphology, surface energy and crystallinity and photovoltaic characteristics were studied.

Poster Presentation : **MAT.P-588**

Material Chemistry

Event Hall THU 11:00~13:00

Soft organic optoelectronic synaptic device based on elastomeric materials

Myeonghyeon Na, Kyoseung Sim*

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The organic semiconductor-based electronic devices exhibiting artificial synaptic behavior are in the spotlight as promising potential future electronics for neuromorphic computing applications. Particularly, organic synaptic devices that use optical stimulation for synaptic behavior, commonly called organic optoelectronic synaptic devices, enable high-speed communication, low cross-talking, high bandwidth, ultra-low energy consumption and etc. Moreover, soft optoelectronic synaptic devices with all elastomeric materials provide substantial advantages for future wearable electronic systems due to mechanical conformability and comparability to the soft human bodies. Here, we proposed fully soft optoelectronic synaptic devices based on organic semiconductors with a simple structure. Various essential synaptic behaviors by optical stimulation were characterized and the devices show stable operation under mechanical strain.

Poster Presentation : **MAT.P-589**

Material Chemistry

Event Hall THU 11:00~13:00

Superior Heavy Metal Ion Adsorption Capacity from Water by High-density Thiol Functionalized Reduced Graphene Oxides

Seon Kyeong Kim, Ki-Wan Jeon[1,*]

Energy & Applied Chemistry, Silla University, Korea
[1]*Department of Environmental Energy & Chemistry, Silla University, Korea*

Reduced graphene oxy-sulfide (mRGO) obtained using P_4S_{10} as thionating agent via a facile solvothermal reaction has come out as a potential absorbent for scavenging heavy metal ions (Pb^{2+}, Hg^{2+}, Cd^{2+}), especially Pb^{2+}, from aqueous solution due to the presence of thiol (-SH) functional groups. The existence of –SH groups was further verified by X-ray photoelectron (XPS) studies. The highest adsorption capacity of Pb^{2+} ions on the mRGO surface was around 858 mg/g at pH 7, 25 °C. Furthermore, it was found that the adsorption of Pb^{2+} onto mRGO was influenced by a change in the pH 7 from acidic to the basic range. Time-dependent (percentage) % Pb^{2+} ions removal study also shows promising results. Almost 95 % removal of Pb^{2+} ions was achieved within 30 min at pH 7 and 25 °C using 1 ppm Pb^{2+} solution as a test solution. This study clearly indicates the potential and efficient utilization of this new functionalized carbonaceous material for removing environmentally benign Pb^{2+} from groundwater.

Poster Presentation : **MAT.P-590**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and Characterization of Phosphine Oxides and Triazine Derivative for Enhanced Mobility and Restricted Traps in Electron Transporting Layers

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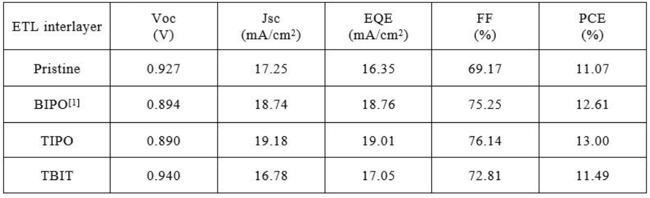
Department of Materials Engineering and Convergence Technology, Gyeongsang National University, Korea

[1]Department of Chemistry, Gyeongsang National University, Korea

Tris(4-(1-phenyl-1H-benzo[d]imidazole)phenyl)phosphine oxide (TIPO) and Tris(4-(1-phenyl-1H-benzo[d]imidazole)phenyl)triazine (TBIT) were newly synthesized and applied to n-type interlayer of planar perovskite solar cells (PSCs) for effective electron transport layer. The molecule materials contained phenyl benzimidazole group which is combined with a phosphine oxide core or triazine ring core and has contributed to the improvement of charge extraction and stability. Since the constituent molecules phosphine oxide and benzimidazole (BIZ) have high polarity and strong π-electrons, the molecules trigger passivation defects to improve charge transport and flattening the surface morphology. In addition, the stability of the device was improved by introducing TIPO material as the passivation and protection layer.

Table 1. Photovoltaic parameters of device with BIPO, TIPO, and TBIT interlayers.



ETL interlayer	Voc (V)	Jsc (mA/cm^2)	EQE (mA/cm^2)	FF (%)	PCE (%)
Pristine	0.927	17.25	16.35	69.17	11.07
BIPO[1]	0.894	18.74	18.76	75.25	12.61
TIPO	0.890	19.18	19.01	76.14	13.00
TBIT	0.940	16.78	17.05	72.81	11.49

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-591**

Material Chemistry

Event Hall THU 11:00~13:00

Soft optoelectronic devices enabled by elastic light absorption layer consisting of a p-n junction

Sehyun Kim, Kyoseung Sim*

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Organic optoelectronic devices have been developed considerably recently because of their crucial advantages such as light-weight, mechanical softness, low-cost manufacturing, etc. For future wearable electronics, for example, skin-mountable electronics, artificial vision systems, optical communications, etc. Especially, Organic photodetector is one of the essential sensing components for the various optoelectronic systems. Therefore, the development of soft organic photodetectors provides a better route to achieve the demonstration of the wearable electronic system. Here, we propose a fully soft photodetector based on elastic light absorption layer that is composed of a p-n junction by polymeric semiconductors. Depending on the composition of the light absorption layer, the fabricated devices' performance and origin of performance variation were characterized and investigated, respectively. In addition, the demonstrated soft organic optoelectronic devices show stable operation under mechanical strain, which could be a promising candidate for future electronic devices.

Poster Presentation : **MAT.P-592**

Material Chemistry

Event Hall THU 11:00~13:00

The lithium ion conductor of calcium substituted Li-Sn-S system

Seung-Tae Hong*, Seo Hyeonjin[1,*]

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Lithium ion conducting solid electrolytes show promise for enabling high-energy secondary battery chemistries and solving safety issues associated with conventional lithium batteries. Solid electrolytes may reduce the safety issues associated with liquid-based electrolytes and improve the compatibility with anode and cathode materials over a range of cell voltages. Li-Sn-S system is an air-stable thio-LISICONs solid electrolyte and has a ionic conductivity of 7.0 x 10-5S/cm (In this work, it has 1.98 x 10-6S/cm). To improve ionic conductivity by replacing Li cation with Ca cation, the solid electrolyte of composition Li-Ca-Sn-S system was synthesized by solid state synthesis method. The ionic conductivity continued to increase while substituting Ca cation, and showed a maximum value of 1.23 x 10-5S/cm at C=0.25. This is an increase of about 10 times compared to the previous value. Thereafter, the ionic conductivity decreases at C>0.25, which is expected due to the impurity related to precursor. As a result of the XRD pattern, there are no structural change was observed when substitution occurred. The lattice parameter of L-C-S-S C=0.25 was slightly larger than that of L-S-S system, indicating that substitution of a Li cation by the larger Ca cation enlarged the lattice. This is also consistent with the activation energy tendency. Through the discovery of this material, a strategy for improving ionic conductivity through Li vacancy can be established.

Poster Presentation : **MAT.P-593**

Material Chemistry

Event Hall THU 11:00~13:00

Thermoelectric properties of Ag-doped polycrystalline SnSe

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[1]*School of Chemical & Biological Engineering, Seoul National University, Korea*

Thermoelectric materials can provide an effective and eco-friendly solution to global energy and environmental crises because it can harvest waste heat and convert into a useful form of electrical energy. SnSe material has intrinsically favorable electronic and phonon structures, thereby showing extraordinarily high thermoelectric performance. However, it has been only observable in properly prepared single crystal samples. Because high quality single crystal samples require a lot of time and cost and they are mechanically fragile, realizing comparable or even higher thermoelectric performance in polycrystalline sample has been a core task in the thermoelectric society. In this presentation, we report the effects of Ag doping on charge and thermal transport properties of polycrystalline SnSe. Ag doping improves the power factor due to the increase in the Seebeck coefficient and decreases the thermal conductivity. As a result, the optimal composition shows a thermoelectric figure of merit, ZT, of 1.2 at 800K.

Poster Presentation : **MAT.P-594**

Material Chemistry

Event Hall THU 11:00~13:00

Fe3C/N-doped carbon hybrid materials for oxygen evolution reaction electrocatalysts

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Inha University, Korea

[1]*Department of Chemistry, Inha University, Korea*

Electrochemical water splitting is an important process for next generation of eco-friendly energy systems. The oxygen evolution reaction (OER) occurs at an anode during the process and requires efficient electrocatalysts to reduce activation energies. Ru or Ir-containing materials have proved its best catalytic activities; their high cost is a critical drawback. Therefore, it is necessary to develop efficient electrocatalysts composed of low-cost metal components. Herein, a hybrid material (Fe-NC) containing Fe3C particles dispersed on the surface of N-doped carbon materials was synthesized by heat treatment of a mixture of urea and Fe(II)Cl2(H2O)4. Microscopic analyses and various characterizations reveal that the Fe3C particles are placed on the surfaces of thin NC materials. The Fe-NC exhibit superior electrocatalytic performance with onset and over-potentials of 1.57 V and 545 mV for OERs in a basic media. This study suggests the possibility of the use of Fe3C-based composites as OER electrocatalysts.

Poster Presentation : **MAT.P-595**

Material Chemistry

Event Hall THU 11:00~13:00

Stretchable Liquid Metal / Block Copolymer Multilayer for Moisture Encapsulation

Salma Faiz, Seunggoo Baek, Unyong Jeong*

Materials Science and Engineering , Pohang University of Science and Technology, Korea

Gas and moisture have a direct influence on the performance of electronic devices. Encapsulation barriers are critical for a proper application. In this study, we suggest a stretchable moisture encapsulation with the organic-inorganic multilayer structure for stretchable devices. Poly(styrene-b-isobutylene-b-styrene) copolymer (SiBS) and Eutectic-GaIn liquid metal (LM) were used as the organic and inorganic layers, respectively. The intrinsic stretchability of the LM layer reduces the moisture penetration, which improves the barrier property, while preserving the stretchability of the multilayer encapsulation. The 4 layers encapsulation exhibits low water evaporation rate of 12.5 μg/h and is stretchable up to 50% uniaxial strain. We deploy this multilayer barrier to provide effective encapsulation to an ionic-gel based temperature sensor under humid conditions (Relative humidity of 90%) for 100h.

Poster Presentation : **MAT.P-596**

Material Chemistry

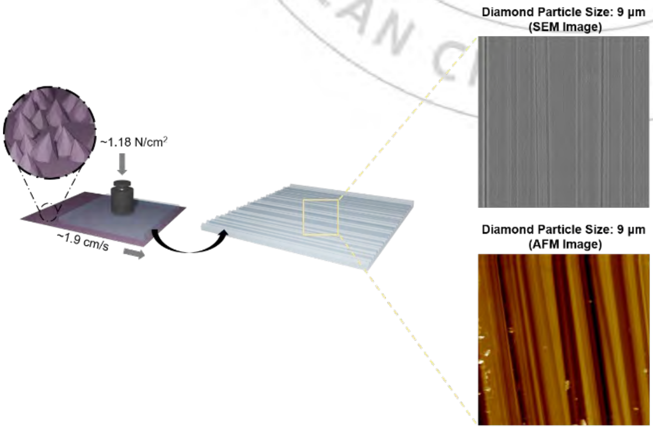
Event Hall THU 11:00~13:00

Fabrication of Scratched Nanogroove for Highly-Ordered Cell Alignment

<u>Baekman Kim</u>, Dong Ki Yoon*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Transplantation has grabbed significant attention as damaged organs and tissues require medical treatments. Yet, numerous attempts to reconstruct organs and tissues were unsuccessful due to inflammatory immune response and compatibility between donor and recipient. Herein, we propose the fabrication of a cell-alignment scaffold that can enhance cell growth, accelerate proliferation, and reproduce cellular arrangement in native tissue. The fundamental is scratching a diamond lapping film that affords uniaxial nanotopography on various substrates. Cells seeded on a nanotopography then guide themselves following the geometric cue via contact guidance, resulting in aligned growth and migration. Further functionalization with poly(N-isopropylacrylamide) (pNIPAM) promotes cell sheet detachment. We believe that our method will be widely applied in bioengineering, tissue engineering, and therapeutic purpose.



Poster Presentation : **MAT.P-597**
Material Chemistry
Event Hall THU 11:00~13:00

Unidirectionally Oriented DNA-Based Hydrogel through Unpolarized Light Scanning

Juri Kim, Dong Ki Yoon*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Hydrogel is a three-dimensionally crosslinked polymer network, and its water-rich and soft mechanical properties are similar to biological tissues. Because of these properties, it has been spotlighted in the biomedical field. However, the structure and properties of the fabricated hydrogels are different from those of in vivo tissues. In generally, it is due to the isotropic gelation process of the polymer network, which is different from the hierarchical structure of living tissues. In order to mimic anisotropy of tissues, studies on fabrication of anisotropic structures using various forces and equipment, including shear force, electromagnetic fields, and lithography, have been reported. However, a limitation of these studies is that the fixation process is required after oriented or that they needed two or more steps. Herein, we fabricated a patterned or unidirectionally oriented hydrogel in one step by controlling the diffusion of the photopolymerizable monomer through light. The orientation of the hydrogel could be freely controlled according to the light irradiation area since DNA which forms physical gelation complex with polymerized chain is in liquid crystalline phase, and contraction & tensile force occur due to diffusion of monomer. Expanding on this concept, it was possible to fabricate uniaxially oriented hydrogels without dye molecule through unpolarized light scanning. Moreover, the fabricated hydrogel can control its shape reversibly through hydration/dehydration process and has an orientation memory effect that allows it to return to its original orientation. The fabricated hydrogel has various advantages, and it seems that it can be applied in various ways.

Poster Presentation : **MAT.P-598**

Material Chemistry

Event Hall THU 11:00~13:00

Heteroatom-containing Fluorinated Porous Organic Polymer for High-Performance Sulfur Cathodes in Lithium-Sulfur Batteries

Doyun Kim

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Lithium−sulfur (Li−S) batteries by far offer higher theoretical energy density than that of the commerciallithium-ion battery counterparts, but suffer predominantly from an irreversible shuttling process involving lithium polysulfides. Here, we report a heteroatom-containing fluorinated covalent organic polymer (F-COP) as a template for high-performance sulfur cathodes in Li−S batteries. The fluorination allowed facile covalent attachment of sulfur to a porous polymer framework via nucleophilic aromatic substitution reaction (SNAr), leading to high sulfur content, e.g., over 70 wt %. The F-COP framework was microporous with 72% of pores within three well-defined pore sizes, viz. 0.58, 1.19, and 1.68 nm, which effectively suppressed polysulfide dissolution via steric and electrostatic hindrance. As a result of the structural features of the F-COP, the resulting sulfur electrode exhibited high electrochemical performance of 1287.7 mAh g^{-1} at 0.05C, 96.4% initial Columbic efficiency, 70.3% capacity retention after 1000 cycles at 0.5C, and robust operation for a sulfur loading of up to 4.1 mg_{sulfur} cm^{-2}. Our findings suggest the F-COP family with the adaptability of SNAr chemistry and well-defined microporous structures as useful frameworks for highly sustainable sulfur electrodes in Li−S batteries.

Poster Presentation : **MAT.P-599**

Material Chemistry

Event Hall THU 11:00~13:00

Photo-controlled Capacitor based on Photo-responsive Dielectric Nanocomposites

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[1]*School of Integrated Technology, Yonsei University, Korea*

Light is an attractive stimulus in that it allows a remote spatio-temporal control. Therefore, photo-responsive materials and devices have been actively studied. For example, Au nanorod (AuNR) array-embedded polymers (e.g., polydimethylsiloxane (PDMS), and polystyrene) doped with various azobenzene derivates (e.g., azobenzene, *p*-hydroxyazobenzene, and *p*-aminoazobenzene) exhibited changes in dielectric properties upon irradiation of UV light, which can be applied to a photo-controlled capacitor.In order to enhance the dynamic range of the dielectric material's dielectric strength, we chemically incorporated azobenzene into the high molecular polymer instead of physical doping. Accordingly, we developed a photo-controlled capacitor composed of a high-dielectric two-dimensional AuNR array embedded in photo-responsive dielectric polymer matrix (azobenzene-incorporated PDMS; AzoPDMS). The dielectric strength of AzoPDMS matrix is controlled via cis-to-trans photoisomerization upon irradiation of 400 nm – 700 nm light, while the NR array surrounded by polymer matrix acts as conductive pathways preventing the material from irreversible dielectric breakdown simultaneously. Our photo-controlled capacitor can be utilized in light-modulated electronics such as a conductor-dielectric switch, or in predicting materials’ chemical arrangements via monitoring real-time electric signals.References J. Kim, B. A. Grzybowsk, Advanced Materials 24. 14 (2012).

Poster Presentation : **MAT.P-600**

Material Chemistry

Event Hall THU 11:00~13:00

Low voltage electrowetting valve in microfluidic devices using low-cost commercial Cu films

Hyuckjin Lee, Oh-Sun Kwon, Kwanwoo Shin*

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POCT devices used for on-site diagnosis of diseases should be small in size for portability, low-cost for easy mass production, and simple in fabricating process. These microfluidic-based devices often use electrowetting to control the fluid using voltage. The existing low-voltage E-valve is fabricated by printing conductive Ag ink, so it is expensive, and the process is complicated. Therefore, we devised a low-voltage E-valve that is low-cost and simple to fabricate using commercial copper film with a thickness of 70um. Hydrophobic coating of copper film is possible by washing the film in 1M HCl solution for a few seconds, calcinating at 400°C for 3 hours, and immersing it in 1.0 v/v PFDT solution for 10 minutes. The contact angle on the PFDT-coated hydrophobic copper film is about 122 degrees, which is similar to the hydrophobic coating used for general electrowetting, and the PFDT-coated hydrophobic copper valve can stop the flow of fluid for up to several hours. This valve can be opened within a few seconds with a battery-level voltage of less than 40v, there is no fluid leaking or clogging common to microfluidics devices, and the durability of the coating also lasts for several months. Based on these results, it will be possible to easily control the microfluid at low voltage using an inexpensive copper film in POCT.Keywords: microfluidics, continuous microfluidics, electrowetting, low voltage, Lab-on a chip

Poster Presentation : **MAT.P-601**

Material Chemistry

Event Hall THU 11:00~13:00

A Simple Method for Synthesizing Ge/GeO$_2$/Titanate Nanosheet composites as High-Stability Anode Materials for Li-Ion batteries

Dongjun Park, **Seung-Min Paek**[1,*]

chemistry, Kyungpook National University, Korea
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Recently, Li-ion batteries have been used in various devices and electric vehicles as electrochemical charge devices. In this experiment, Ge/GeO$_2$ nanoparticles were used as anode materials for Li-ion batteries. The battery assembled using Ge/GeO$_2$ nanoparticles has a large initial charge/discharge capacity, but the capacity continues to decrease and the capacity cannot be maintained. To solve this problem, Ge/GeO$_2$ nanoparticles were dispersed and TBA-titanate was synthesized. As a result of synthesis, the initial charge/discharge capacity was reduced compared to the assembled battery by dispersing only the Ge/GeO$_2$ nanoparticles, but as the cycle went on, the reduced capacity became smaller and the capacity was better maintained. It was also synthesized with different ratios of Ge and TBA-titanate. The higher the amount of Ge, the larger the initial capacity and the lower the capacity maintenance. But the smaller the amount of Ge, the smaller the initial capacity, and the capacity was maintained better because the volume change effect decreases by synthesizing TBA-titanate.

Poster Presentation : **MAT.P-602**

Material Chemistry

Event Hall THU 11:00~13:00

Adsorptive removal of small cationic dyes with oxidatively modified metal-organic framework-derived carbons

Md abul Hossain, Sung Hwa Jhung*

Department of Chemistry, Kyungpook National University, Korea

Removal of organic dyes from wastewater is very important for our safe environment and sound health. In order to improve the performance of metal-organic framework (MOF)-derived carbons (MDCs) in dye adsorption, an MDC, derived from MAF-6, was oxidatively modified with ammonium persulfate solutions (APSs). Although the porosity of pristine MDC decreased with oxidation, oxidized MDCs (OMDCs), especially OMDC(1.0), that was obtained via treating MDC with 1 M APS, showed remarkable performances in adsorption of small cationic dyes like methylene blue (MB) and azure B. For example, OMDC(1.0) had the maximum adsorption capacity of 625 mg/g (for MB) which is larger than any reported value with carbonaceous materials. On the contrary, oxidative treatment of MDC was negative in adsorption of anionic dye such as methyl orange. Moreover, oxidized MDC was not very effective in adsorption of cationic dyes with large size (like brilliant green, crystal violet, Janus green B and rhodamine B) because of limited pore size of the studied adsorbent OMDC(1.0). The remarkable adsorption of MB over OMDC(1.0) could be explained with electrostatic and π–π interactions. Finally, the facile recyclability of the OMDC(1.0) in MB adsorption was confirmed via successive adsorptions, FTIR, and nitrogen adsorption; therefore, OMDC(1.0) can be suggested as a potential adsorbent to remove cationic dyes, especially with small molecular sizes. Keywords: adsorption; dye removal; mechanism; MOF-derived carbon; oxidized carbon

Poster Presentation : **MAT.P-603**

Material Chemistry

Event Hall THU 11:00~13:00

Role of Surface Wettability in High-Throughput Liquid Metal Printing Based Fabrication of Molecular Junction Arrays

Seo Eun Byeon, Gyu Don Kong, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

If molecular electronics can be merged with printed electronics, it can allow reliable and economical mass production of molecular-scale electronic devices for practical applications. It is, however, difficult to achieve such a goal because direct printing of electrode onto one-nanometer-thick organic films (i.e., monolayers) in a noninvasive manner and with high regularity remains challenging. This presentation shows that high-throughput liquid metal printing based fabrication of molecular junction arrays is significantly influenced by surface wettability of liquid metal electrode over ultraflat substrates whose surface is mostly hydrophobic due to use of organic polymer-based optical adhesive during template-stripping process. Our experiments reveal that the surface wettability determines the regularity of printed liquid metal electrodes, which is directly translated into dispersion of current density values and yield of working junctions. Our work represents an important step toward printed molecular electronics.

Poster Presentation : **MAT.P-604**

Material Chemistry

Event Hall THU 11:00~13:00

Molecular Mix Suppresses Thermopower of Molecular Junctions

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[1]*Department of Chemistry, Korea University, Korea*

With recent developments in nanotechnologies, waste heat management in nanoscale materials and devices has emerged as an important issue. Molecular thermoelectrics aims to explore heat-to-electricity conversion on a molecular scale. Most studies in molecular thermoelectrics have focused on enhancing thermopower of molecular-scale devices, yet little is known about how to suppress it. This presentation describes a study that compares Seebeck coefficient between pure and mixed self-assembled monolayers (SAMs) and reveals significantly reduced Seebeck coefficient in mixed SAM. Specifically, we measured Seebeck coefficient of pure SAMs of *n*-butanethiol and 11-mercaptoundecanoic acid molecules and their mixed SAMs. Our experiments reveal that the molecular mix induces supramolecular disorder, which suppresses the thermopower of the molecular junction. Our work demonstrates that control over supramolecular structure within monolayers plays a critical role in the thermoelectric performance of molecular junction.

Poster Presentation : **MAT.P-605**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and Characterization of Organoboron Material for Blue Thermally Activated Delayed Fluorescence

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Chemistry, Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*

A number of studies about TADF have been proceeding and organoboron materials have exhibited high performance when they are fabricated for emitters of OLED. Among these, materials having multiple-resonance (MR) induced by introducing nitrogen or oxygen atoms into core skeleton have more improved efficiency than preceding things in terms of quantum yield, TADF lifetime, and kRISC value. Here, we report new multiple-resonance organoboron material for blue TADF. The core structure was synthesized by lithiation, and we introduced the substituents to adjust the properties such as emission wavelength. 1H-NMR, UV-Vis and PL spectroscopy, and cyclic voltammetry were carried out for characterization.

Poster Presentation : **MAT.P-606**

Material Chemistry

Event Hall THU 11:00~13:00

Surface characterization and drug release behavior of S-doped TiO_2 and MoS_x coating layers on Ti-Mo alloys

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Heterogeneous layer structures consisted of S-doped TiO2 and MoSx particles were prepared on the Ti-Mo alloys (Mo : 2.5 ~ 15 wt%) and the drug materials were adsorbed in their layer structures for dental implant surface treatment. The layer properties and release behaviors were investigated. Heterogeneous layer structures were hydrothermally synthesized on Ti-Mo alloys with Na2S dissolved in 0.4 M HCl solution at 225 °C. S-doped rutile TiO2 nanorods for Ti-rich areas and hexagonal and metallic MoSx nanoparticles (2H-MoS2 and 1T-MoS2) for Mo rich area were observed after hydrothermal treatment of Ti-Mo alloys. When the Mo content in Ti-Mo alloy was increased by more than 10 wt%, metallic MoS2 was mainly formed compared to hexagonal MoS2 In this study, heterogeneous layer structures were used as drug delivery system. Vancomycin was applied to these layer structures protecting bacterial infections and the release behavior was investigated using the real-time analysis Raman method.

Poster Presentation : **MAT.P-607**
Material Chemistry
Event Hall THU 11:00~13:00

Nanocrystalline beta zeolite-supported CoMo catalyst for hydroprocessing of methyl palmitate to bio-jet fuels

Sangwook Kang, Kyoungsoo Kim[1,*]

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Catalytic hydroprocessing comprising hydrodeoxygenation, hydrocracking and hydroisomerization is a key technology for bio-jet fuel production. Here, we synthesized highly selective CoMo catalyst to bio-jet fuel, using nanocrystalline beta zeolite as a support. Cyclic diammonium having structure-directing ability for beta zeolite structure was used to prepare the zeolite support. The synthetic zeolite consisted of nanocrystals with a diameter of approximately 15 nm, thereby having large external surface area (330 m^2 g^{-1}) and intercrystal mesoporosity. The contents of silanol groups in the zeolite could be adjusted by changing basicity of the synthetic gel. CoMo nanoparticles were impregnated into three types of zeolite: one commercial bulk beta zeolite and two nanocrystalline beta zeolites with low and high silanol content. Electron microscopic observation showed that the nanoparticles were located on the external surfaces of zeolite supports. Accordingly, the particle dispersion was higher in the case of using nanocrystalline zeolites possessing larger external surface area than bulk zeolite. X-ray photoelectron spectroscopic studies revealed that the zeolite silanol helped CoMo to form more reduced phase. In hydroprocessing of methyl palmitate, the CoMo catalyst supported on the nanocrystalline zeolite with a lot of silanol groups exhibited the highest yield to iso-paraffin with a C_8-C_{16} carbon number range (i.e. jet fuel fraction) among the three catalysts. The best performance was attributed to synergetic combination of the zeolite mesoporosity and the reduced state of CoMo catalyst. Furthermore, this catalyst also showed high selectivity to bio-jet fuel fraction in upgrading of commercially available bio-diesel through catalytic hydroprocessing.

Poster Presentation : **MAT.P-608**

Material Chemistry

Event Hall THU 11:00~13:00

Phosphorescent Near-Infrared Iridium(III) Complex Overcoming Energy-Gap Law by Intermolecular Charge Transfer

Hae Un Kim, Jihyun Min, Taiho Park*

Department of Chemical Engineering, Pohang University of Science and Technology, Korea

Efficient organic near-infrared (NIR) emitters are needed especially for deformable light-emitting devices, especially for their ability to penetrate body tissue. However, by the energy-gap law, the non-radiative decay rate increases exponentially as the bandgap energy decreases. There is a need to overcome the weak luminescence of NIR OLEDs. NIR emissive Iridium(III) complexes with different electron-withdrawing abilities on the (benzo[*b*]thiophen-2-yl)quinoline ligand were designed and synthesized. Intermolecular charge transfer mechanism facilitated by aggregation-induced phosphorescent enhancement (AIPE) effect achieves maximum external quantum efficiency (EQE) of 7.29%. The results give promising NIR phosphorescent dopant design strategies.

Poster Presentation : **MAT.P-609**
Material Chemistry
Event Hall THU 11:00~13:00

Ni-Ce alloy supported on mesoporous silica as a bimetallic catalyst for dry reforming of methane

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Department of Chemistry, Sungkyunkwan University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, China*

The dry reforming of methane (DRM; $CO_2 + CH_4 \rightarrow 2CO + 2H_2$) is attracting attention as a reaction to generate valuable synthesis gas using greenhouse gases, as an increase in concern for reduction and utilization of greenhouse gases. Nickel is most widely used as a catalyst for reforming, but the high reaction temperature of DRM causes aggregation of the catalysts and severe coke formation leading to deactivation.In this study, we prevented the sintering and coking by impregnating Ni and Ce nanoparticles into the mesoporous silica support. Cerium can increase the dispersion of Ni nanoparticles and stabilize catalyst during the reaction. The dispersion of the active site after thermal activation as well as the catalytic activity and stability of the catalyst after reduction will be presented.The synthesized catalytic properties were analyzed by X-ray diffraction (XRD), nitrogen adsorption and desorption isotherms, scanning electron microscope (SEM), transmission electron microscope (TEM), and temperature programmed reduction (TPR).

Poster Presentation : **MAT.P-610**

Material Chemistry

Event Hall THU 11:00~13:00

Efficient Bimetallic Catalysts for Ethane Oxidative Dehydrogenation using CO_2 as Soft Oxidant

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Ethane oxidative dehydrogenation in presence of CO_2 for ethylene production is an appealing route. Using CO_2 as oxygen supplier for removal of hydrogen, resulting value-added basic chemicals through oxidative dehydrogenation. Zeolite supported Pt based bimetallic catalysts were prepared with rare earth metals (La, Sc, Y) as second metal. The catalysts were characterized using X-ray photon spectroscopy, STEM, TEM, CO-chemisorption, TGA, XRD and ICP-OES. From TEM data, it was found that among all samples, catalyst having La as second metal (Pt-La@ZNS) gave better Pt dispersion with average particle size of 1.25nm. All the catalysts were examined for ethane oxidative dehydrogenation to ethylene in CO_2 as soft oxidant. Reaction parameters were optimized. The activity and life span of catalysts were increased with REE addition. During dehydrogenation, CO_2 contributes in enhancement of dehydrogenation activity through reverse water-gas shift reaction. Moreover, CO_2 can react with surface carbon formed that help in removal of coke through reverse Boudouard reaction.

Poster Presentation : **MAT.P-611**

Material Chemistry

Event Hall THU 11:00~13:00

Surgical Suture Engineered with an Extracellular Matrix

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Surgical suture is a medical device used to hold injured tissues together after operation. It often brings undesired infection or secondary wound due to the friction at the interface between the tissue and the suture. In this research, we designed fibronectin (FN)-coated suture using UV/ozone (UVO) irradiation or polystyrene sulfonate acid (PSS) dip-coating where FN plays crucial role in wound healing as an extracellular matrix compound. This improves cellular activity around the damaged tissue to prevent bacteria from binding. Moreover, it is found that FN-coated suture has lower friction compared to the commonly used device which will minimize secondary trauma. Based on the research, the method can be further applied to engineer other beneficial proteins to produce suture for different purposes.

Poster Presentation : **MAT.P-612**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation of porous expanded graphite for high-performance hydrogen storage by peroxide treatment.

YeongHun Kim, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

This study analyzed the room temperature hydrogen uptake capacity of expanded graphite produced when graphite flakes were treated with peroxide. Expanded graphites with high porosity were synthesized by sulfuric acid and hydrogen peroxide. The graphite flakes were ground by disk millimg and sieved. After sieved, graphite flakes treated by phiranha solution. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns. The N2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 60 bar.

Poster Presentation : **MAT.P-613**

Material Chemistry

Event Hall THU 11:00~13:00

Vapor-Induced Fluorochromic Material Based on Naphthalene Diimide for Efficient Volatile Organic Compounds Detection

Gwiung Nam, Min-Ji Kim, Kyung-Ryang Wee*

Department of Chemistry, Daegu University, Korea

A series of naphthalene diimide (NDI) acceptor (A) and triphenylamine donor (D) based D–A–D systems were designed and synthesized for the efficient detection of volatile organic compounds (VOCs). To investigate the correlation between the isomer effect and vapofluorochromism, D–A–D system was comprised of *ortho*-, *meta*-, and *para*-position isomer compounds (**NDI-TO**, **NDI-TM**, and **NDI-TP**). The emission spectra of all compounds exhibited a red-shift with increasing solvent polarity, indicating the presence of an intramolecular charge transfer (ICT) state in the excited state. However, the thin film emission spectra of all compounds show quenching of emission in the solid state. These results indicate that the emission is quenched by the intermolecular interaction. Based on these properties, all compounds showed emission activation and vapofluorochromism by vapor stimulation of VOCs in the thin film state. Initial compounds in the thin film state exhibit quenched emission due to strong intermolecular interaction. Exposure to vapors under these conditions increases the distance between molecules and decreases intermolecular interactions leads to the single molecular ICT emission. Furthermore, as the polarity of the VOCs increased, the emission color was red-shifted. This result means that the VOCs can be distinguished by the change of the emission color. In particular, among the isomers, π-conjugation-breaking systems of **NDI-TO** and **NDI-TM** expanded the emission region of vapofluorochromism more than π-conjugated **NDI-TP**. These results suggest that the non-π-conjugated system has a larger change in emission spectrum according to the polarity of VOCs than the π-conjugated system, which facilitates the detection of VOCs.

Poster Presentation : **MAT.P-614**

Material Chemistry

Event Hall THU 11:00~13:00

Efficiently Controllable Mechanofluorochromic Material Based on Pyrene 2,7-Position Substituted Donor–Acceptor–Donor System

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We report on the mechanofluorochromic (MFC) activation of donor–acceptor–donor (D–A–D) pyrene (Py) 2,7-position-based compounds by facile intra- and intermolecular charge transfer control via the electron push-pull effect of the functional R group. For these compounds, as the electron-withdrawing ability of the substituent R increases, the intramolecular interactions become insufficient and induce strong intermolecular donor–acceptor (D–A) interactions for stabilizing molecules, leading to MFC activation. On the other hand, as the electron-donating ability of the substituent R increases, the intramolecular interaction is enhanced and induce weak intermolecular D–A interaction leading to MFC inactivation. In other words, the MFC material has more limited emission in the long wavelength region than the emission in the short wavelength region of blue and green. Therefore, based on these results, we further report MFC-activating materials for controlling a wide range of emission colors. In the Py 2,7-position-based compounds, a cyanide substituent for MFC activation is introduced at one of the two para-position of the donor molecule and an R group for fine control of emission color is introduced at the other site. These compounds showed MFC properties even when the electron-donating ability of the substituent R was increased, and the emission color was also finely controlled.

Poster Presentation : **MAT.P-615**
Material Chemistry
Event Hall THU 11:00~13:00

Doping and Thermoelectric Behaviors of Donor-Acceptor Polymers with Extended Planar Backbone

Subin Lee, Doyeong Choi[1], Yun Hi Kim[2,*]

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[2]*Department of Chemistry, Gyeongsang National University, Korea*

Thermoelectric (TE) materials are receiving increasing attention due to their ability to directly converting heat to electricity. Polymer-based TE materials are particularly fascinating to wearable and mobile devices due to their low density, good flexibility, and low toxicity. The design of a conjugated polymer backbone influences the charge transport and doping efficiency; however, the construction of the polymer backbone for maximized thermoelectric performance is still unclear. Herein, a novel synthesis of a donor-acceptor (D-A) conjugated polymer with an extended planar backbone, C6-ICPDPP, is reported for the investigation of the thermoelectric behavior. The C6-ICPDPP films are formed from two types of solvents with different boiling points, both of which are doped with $FeCl_3$, showing good thermoelectric properties. The thin-film structure, dopant diffusion, and thickness of the C6-ICPDPP films were different between the two solvents. The optimized power factors are 1.32 $\mu W/mK^2$(p-type) and 0.410 $\mu W/mK^2$ (n-type), respectively, which are consistent with the change in the polaronic features at the given $FeCl_3$ doping concentration. This study provides a design strategy for D-A conjugated polymers with extended planarization and electrical behavior suitable for organic thermoelectrics.

Poster Presentation : **MAT.P-616**

Material Chemistry

Event Hall THU 11:00~13:00

A study of coffee bean wastes-derived activated carbons for hydrogen storage

<u>YeongHun Kim</u>, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this study, porous carbons with high porosity were synthesized by coffee bean waste precursor. The precursors were carbonized at 900°C, 1 hr, and N2 flow conditions using coffee bean waste precursor. After carbonized, porous carbons were synthesized by chemical activation. The effect on quantity of activation reagents was investigated by experience of carbon precursor/chemical reagent mass ratio. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns. The N2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 60 bar.

Poster Presentation : **MAT.P-617**

Material Chemistry

Event Hall THU 11:00~13:00

Burn-in Loss Inspection in Ternary Organic Photovoltaic System Composed of Environmentally Friendly Solvent Processed Semiconducting Polymers and Non-fullerene Acceptor

Dasol Chung, Yelim Choi, Taiho Park*

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UV-crosslinked semiconducting polymer (P2FBTT-Br) and a non-fullerene acceptor (IEICO-4F) in ternary organic photovoltaic system were processed with environmentally friendly solvent and were inspected in this work. UV irradiation was exposed on P2FBTT-Br for 150 seconds for crosslinking and 2-methylanisole dissolved it. Performance test for photovoltaics was executed at 75 °C or AM 1.5G Sun illumination for 90 h, UV-crosslinked devices with PC71BM exhibited 9.2% power conversion efficiency (PCE) and better stability on burn-in loss compared to the pristine cells. Tightly fixed morphology due to the crosslinking constrains post-crystallization and post-aggregation leading to morphological degradation in solar cell devices. When IEICO-4F was used as a non-fullerene acceptor, the burn-in caused by temperature and light was efficiently decreased due to the fixed morphology and high miscibility of the non-fullerene acceptor (18.7% → 90.8% after 90 h at 75 °C and 37.9% → 77.5% after 90 h at AM 1.5G). The resulting crosslinked device exhibited 9.4% PCE (9.8% in chlorobenzene), highest value in crosslinked active materials using environmentally friendly approach.

Poster Presentation : **MAT.P-618**

Material Chemistry

Event Hall THU 11:00~13:00

A Simple Cu(II) Polyelectrolyte as a Method to Increase the Work Function of Electrodes and Form Effective p-Type Contacts in Perovskite Solar Cells

Yohan Ahn

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One effective strategy to improve the performance of perovskite solar cells (PSCs) is to develop new hole transport layers (HTLs). In this work, a simple polyelectrolyte HTL, copper (II) poly(styrene sulfonate) (Cu:PSS), which comprises easily reduced Cu2+ counter-ions with an anionic PSS polyelectrolyte backbone is investigated. Photoelectron spectroscopy reveals an increase in the work function of the anode and upward band bending effect upon incorporation of Cu:PSS in PSC devices. Cu:PSS shows a synergistic effect when mixed with polyethylenedioxythiophene: polystyrenesulfonate (PEDOT:PSS) in various proportions and results in a decrease in the acidity of PEDOT:PSS as well as reduced hysteresis in completed devices. Cu:PSS functions effectively as a HTL in PSCs, with device parameters comparable to PEDOT:PSS, while mixtures of Cu:PSS with PEDOT:PSS shows greatly improved performance compared to PEDOT:PSS alone. Optimized devices incorporating Cu:PSS/PEDOT:PSS mixtures show an improvement in efficiency from 14.35 to 19.44% using a simple CH3NH3PbI3 active layer in an inverted (P-I-N) geometry, which is one of the highest values yet reported for this type of device. It is expected that this type of HTL can be employed to create p-type contacts and improve performance in other types of semiconducting devices as well.

Poster Presentation : **MAT.P-619**

Material Chemistry

Event Hall THU 11:00~13:00

Functionalized Polyvinyl Alcohol Derivatives as Membranes to Increase the Selectivity of Organic Field Effect Transistor Based Chemical-Vapor Sensor

JaeHyun Lee

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Electronic noses(E-noses) are an emerging class of detector that mimic olfactory organs and quantify scents. For commercial success, they must be able to identify a wide range of scent molecules and be manufactured economically. Organic field effect transistors (OFETs) sensors can be fabricated cheaply and in large arrays by economical processes such as ink-jet printing, however, lack selectivity. In this work, we explore the used of semi-permeable membrane polymers by depositing them on top of OFET chemical-vapor sensors, as a method to improve selectivity by selectively allowing desired analytes to pass through and interact with the OFET sensor. A series of acylated poly(vinyl alcohol) (PVA) derivatives is synthesized, characterized and evaluated in OFET vapor sensor as tunable, semi-permeable membranes. Poly(vinyl benzoate), poly(vinyl palmitate), poly(vinyl pivalate), poly(vinyl cinnamate) are synthesized via a microwave-assisted esterification reaction in a facile and economical procedure. OFET vapor sensors are fabricated with and without acylated PVA membranes, and show improved selectivity in the detection of a variety of analytes.

Poster Presentation : **MAT.P-620**

Material Chemistry

Event Hall THU 11:00~13:00

Gas-facilitated One-pot Synthesis of LaOCl:Tb^{3+}Thin Film Fabrication

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[1]*Department of Environmental Energy & Chemistry, Silla University, Korea*

Lanthanum oxychloride phosphor doped with rare earth elements are interesting materials due to easy altering emission light with different doping elements, which can be useful for various application fields. Despite of extensive research of oxychloride-based phosphors, fabrication development of those thin films has rarely studied. Therefore, a systematic study of lanthanum oxychloride thin film could be important due to has potential for light emitting display and gas sensor applications. In this work, we develop for the first time a facile one-step fabrication of LaOCl:Tb^{3+} thin film with spin coating approach. To characterize as-the fabricated thin film, XRD, PL, SEM, TEM, XPS have been conducted. With SEM results, LaOCl:Tb^{3+} was homogeneously distributed with the entire substrate and an estimated thickness of the thin film was about 2 μm. Moreover, XRD and PL results directly indicate that crystallinity and PL intensity of the thin film was strongly depending on heating temperature.

Poster Presentation : **MAT.P-621**

Material Chemistry

Event Hall THU 11:00~13:00

Steam assisted-synthesis of hierarchically porous carbons using mesoporous zeolites as templates

Haneul Yoon, Kyoungsoo Kim*

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Hierarchically meso-/microporous carbons were synthesized using nanocrystalline beta zeolite as a sacrificial template. The zeolite possessed both ordered micropores of the nanocrystals and intercrystalline mesopore voids with 5~15-nm diameters. Various amounts of steam were used with a carbon source, such as ethylene, propylene or acetonitrile, to generate a carbon structure inside the template. The synthesis results showed that adding a suitable amount of steam enabled carbon deposition to be formed selectively inside nanocrystalline zeolites rather than at the exterior by the steam addition. Accordingly, the ordered microporous structure was faithfully replicated into the carbon while the intercrystalline mesopores were retained. Microscopic observation and thermogravimetric analysis revealed that steam oxidized the carbon species deposited at the external surface of zeolite nanocrystals, and hence inhibited the undesirable carbon deposition. Furthermore, such an effect of steam was also applied to the syntheses using other types of mesoporous zeolite material, such as desilicated EMC-2 and USY zeolite, as templates.

Poster Presentation : **MAT.P-622**

Material Chemistry

Event Hall THU 11:00~13:00

GREEN SOLVENT-PROCESSED, HIGH-PERFORMANCE ORGANIC SOLAR CELLS ACHIEVED BY OUTER SIDE-CHAIN SELECTION OF SELENOPHENE-INCORPORATED Y-SERIES ACCEPTORS

Xuyao Song, Bumjoon Kim[1,*], Yun Hi Kim[2,*]

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In this study, we develop three new, green solvent-processable with different outer side-chains ((C3), (C6), and (C9)), affording high-performance OSCs with (o-xylene)-processed active layers. Also, the impact of both outer and inner side-chain engineering of these SMAs on the performance of eco-friendly fabricated OSCs is systematically investigated. The data show that the outer side-chain structure has a much more significant impact than the inner side-chain. The PM6:YSe-C6 blend affords the high-performance OSCs with a power conversion efficiency (PCE) of over 16 %, whereas the PCEs of the YSe-C3- and YSe-C9-based OSCs are only 11-14 %. The lower PCEs of PM6:YSe-C3 and C9 are mainly attributed to reduced electron mobility and increased charge recombination, resulting from aggregate-containing non-optimal blend morphologies. Thus, optimizing the outer side-chain structure of Y-series SMAs is essential for producing green solvent-processed high-performance OSCs.

Poster Presentation : **MAT.P-623**

Material Chemistry

Event Hall THU 11:00~13:00

Quaternary Phosphorus Free Sulfide for Solid-state Electrolyte

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Solid-state electrolytes are emerged as important materials for securing high density, large energy capacity, and stability of batteries. Some sulfur based materials such as $Li_{10}GeP_2S_{12}$(LGPS) and Li_6PS_5Cl(argyrodite) have lithium conductivity similar to or higher than that of liquid electrolytes at room temperature. However, these phosphorus-contained sulfide compounds are sensitive to moisture and air and generate toxic H_2S gas. In this work, we studied phosphorus-free sulfide compound such as $LiGaGeS_4$. Since $LiGaGeS_4$ has defects in cationic site and it is expected that the Li content in the structure can be increased by filling Li in the defect sites through aliovalent substitution. We synthesized $LiGaGeS_4$ by gas-phase synthesis method from oxide analogue $LiGaGeO_4$. Li-ion conductivity and electrochemical properties are measured by electrochemistry impedance spectroscopy(EIS).

Poster Presentation : **MAT.P-624**

Material Chemistry

Event Hall THU 11:00~13:00

Lithium Silicon Nitride as a Sacrificial Electrode Material for Lithium-Ion Batteries

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In LIB, irreversible Li-ion losses due to many side reactions during the initial charging process, which affect the overall capacity. To reduce this capacity loss, sacrificial material with high Li-ion content and low discharge capacity can be used to supply additional Li-ions to the cathode during initial cycle. Various materials such as $LiCoO_2$, Li3N have been reported as sacrificial materials with high chemical and electrochemical stability. In order to increase the capacity, The used of Lithium silicon nitride on first charge has been evaluated electrochemically as and additive electrode material to typical cathode materials. Lithium silicon nitride has been shown to be chemically stable in dry air and can increase the capacity of full-cell.

Poster Presentation : **MAT.P-625**
Material Chemistry
Event Hall THU 11:00~13:00

Aluminum Vanadium Oxide as a Cathode Material for Calcium-Ion Batteries

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Calcium-ion batteries (CIBs) are attracting attention as next-generation batteries. However, there are few cathode materials that intercalate Ca ions reversibly in anhydrous electrolytes. In addition, most of the candidates have problems with the extraction of water molecules, which would make side reactions and not match with Ca-metal. Herein, we report a novel aluminum vanadium oxide (AVO) as a cathode material of CIBs. AVO was synthesized via a facile hydrothermal method. Its structure was first determined from powder X-ray diffraction data(XRD) and the exact atomic ratio was confirmed by Thermogravimetric Analysis(TGA) and X-ray Photoelectron Spectroscopy(XPS). It has a laminar structure with a large interlayer suitable for Ca-ion diffusion having two Al sites and water molecules in the interlayer space per formula unit. Reversible electrochemical intercalation of Ca^{2+} into AVO has been demonstrated using galvanostatic discharge/charge cycling. The reversible discharge capacity is ~116 mAh g^{-1} with an average voltage of 3.18V vs Ca/Ca^{2+}. It showed excellent rate capability and cycle performance. Various analysis tools revealed that aluminum ions and water molecules were not extracted or inserted during the cycle, thereby improving the cyclability. The XRD and Transmission Electron Microscope(TEM) results support small volume expansion thanks to the charge shielding effect of water molecules surrounding the vacant interlayer. The low activation barriers and well-connected diffusion pathway, which is demonstrated by the Bond Vaelence Sum(BVS) calculation, offer insight into the better electrochemical performance and robust structure. This research shows the way for high-energy cathodes in CIBs with reversible cycles.

129th General Meeting of the Korean Chemical Society
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Poster Presentation : **MAT.P-626**

Material Chemistry

Event Hall THU 11:00~13:00

Development of Explosives Simulants for Security Equipment Performance Certification System

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In the field of research, how to evaluate the performance of aviation security equipment is an interesting field. In particular, explosive detection systems(EDS) and explosive trace detection(ETD) that detect explosives require explosives to check the performance of the equipment. In this case, it is safer to use explosive simulant whose stability has been confirmed than an actual explosive. Therefore, in this study, three types of explosive simulants using Petrolatum were developed. The physical characteristics of the simulants were shown through various chemical analyses (TGA, NMR, FT-IR, LC, etc.), and the applicability of actual security equipment was analyzed. Additionally, to increase the reliability of the simulants, analysis of drop tests, friction strength tests, and dust explosion tests is necessary.

Poster Presentation : **MAT.P-627**

Material Chemistry

Event Hall THU 11:00~13:00

Comparison of iodine source materials for red-emitting mixed-halide perovskite QDs

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All-inorganic perovskites (CsPbX3, X=Cl-, Br- and I-) are promissing materials for next-generation display owing to their high color purity, narrow full-width at half-maximum (FWHM), high phtoluminescence (PL) quantum yields and solution processability. Especially, compared to green emission perovskites (CsPbBr3), mixed-halide perovskites for red-emission (600~680 nm) need to adjust the emission wavelength through halide control for pure red-emission (620~640 nm). In general, inorganic materials such as ZnI2 or PbI2 and organic materials such as OAm-I or TMSI have been reported as iodine supply materials for red-emission perovskites. In a previous report, by Kido et al., a mixture of oleylamine (OAm) and iodine (I2) was used as an anion exchange material for synthesis of high efficiency red-emission perovskites. In this work, we synthesized oleylammonium iodide by reacting oleylamine and hydroiodic acid (HI), which was used as an anion exchange material for red perovskite QDs. The chemical, physical and optical characteristics of red perovskite QDs made from our synthesized oleylammonium iodide or the mixture of oleyamine and HI were thoroughly investigated. Furthermore, LED devices were also fabricated, and the results will be discussed in the presentation.

Poster Presentation : **MAT.P-628**

Material Chemistry

Event Hall THU 11:00~13:00

Mesoporous metal oxide catalysts for Preferential Oxidation of CO in H_2-Rich Stream

<u>Zhengyang Li</u>, Chenglin Cui[1], Jung-ho Lee[2], Jin Seo Park[2], Ji Man Kim[2,*]

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The Mesoporous Mn-Co-Ce mixed oxide catalysts were investigated for CO preferential oxidation (CO PROX) reaction, which was synthesized via nano-replication method using a hard template of KIT-6. The catalysts were characterized by X-ray diffraction, N_2 adsorption–desorption, H_2-temperature programmed reduction, CO-temperature programmed desorption and X-ray photoelectron spectroscopy. All of the catalysts had uniform mesopores and high surface areas. The distinct catalytic properties of these well-characterized mesoporous materials were demonstrated for preferential CO oxidation. Among them, the MCC-2 system presented the best CO conversion at low temperatures and the best selectivity toward CO_2. The received mesoporous Mn-Co-Ce mixed oxide possessed excellent textural properties. The structural stability was mainly attributed to the strong and stable interactions between cobalt oxides and manganese oxides.

Poster Presentation : **MAT.P-629**
Material Chemistry
Event Hall THU 11:00~13:00

Mechanochemical synthesis of reduced graphene oxide sheets and their application in supercapacitor electrodes

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We present a one-pot process that can produce highly conductive reduced graphene oxide (RGO) sheets through a mechanochemical method. The synthesis was accomplished by grinding graphene oxide (GO) with solid hydrazine ($H_3N^+NHCO_2^-$), followed by heating the mixed powder at 50 °C The GO sheets were prepared by a simple two-step electrochemical process including the intercalation and oxidation steps. The resulting RGO sheets were fully characterized by X-ray photoelectron spectroscopy, SEM, TEM, Raman spectroscopy, Brunauer-Emmett-Teller measurement, thermogravimetric analysis, and conductivity measurement. They show excellent conductivity and have high specific surface areas. Their electrochemical properties were investigated by cyclic voltammetry, galvanostatic charge/discharge technique, and electrochemical impedance spectroscopy. Details of the experimental results are presented in comparison with RGO sheets prepared using aqueous hydrazine.

Poster Presentation : **MAT.P-630**

Material Chemistry

Event Hall THU 11:00~13:00

A Li-Metal-Pnictogen-Sulfur-Halogen system as a solid electrolyte for all-solid-state batteries

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As the demand for electric vehicles (EVs) and energy storage system (ESS) increase, the development of post-lithium-ion batteries (LIBs) that provide high power, energy density and safety is necessary. Solid electrolyte is an essential component for all-solid-state batteries (ASSBs) which is one of the post-LIBs candidates. Especially, sulfide-based solid electrolyte is well known for its high ionic conductivity, but it is vulnerable for humidity air. To solve that problem, here in, we synthesize Li - Metal(M) - Pnictogen(Pn) – Sulfur - Halogen(X) system(LMPnSX). Additory metal is substituted not only to improve the ionic conductivity but also to reinforce the resistance to air. LMPnSX material is synthesized by solid state method. The presence of impurity and ratio of disordering are demonstrated by X-ray diffraction (XRD). According to electrochemical impedance spectroscopy (EIS), the metal-substituted glass-solid electrolyte shows higher ionic conductivity (~0.6 mS cm-1) than crystalline-solid electrolyte (~0.5 mS cm-1). And both samples show improved ionic conductivity than pristine LMPnSX (~0.1 mS cm-1). The air stability is measured at dryroom (Dew point : -58 ℃). Although exposing the sample in the air for 3 days, there are not noticeable XRD patterns change, and the ionic conductivity is maintained more than ~60% compared with pristine. It means that the LMPnSX system is compatible for air-stable batteries. Also, the further studies about electrochemical cell test with interface stability are required to utilize LMPnSX as the solid electrolyte for ASSBs.

Poster Presentation : **MAT.P-631**
Material Chemistry
Event Hall THU 11:00~13:00

Self-assembly control of Liquid Crystalline Guanine Derivatives

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Molecular self-assembly and crystal structure of liquid crystals (LC) can be adjusted by the molecular structure, heat treatment, additives, etc. LC materials mostly use extensive self-assembly applications on the bulk. Herein, Self-assembly of guanine, mostly studied in small ranges such as DNA strands, was controlled at bulk scale using LC guanine derivatives. guanine-based LC molecules were synthesized containing guanine and peripheral alkoxybenzene part. Ribbon structures or G-quadruplex structures are formed by Hoogsteen hydrogen-bonding and molecules are designed to be adjusted these supramolecular structures depend on the alkyl chain length and the presence of cations. These supramolecular assembly structures show different crystal structures, thermal behavior, and spectroscopy analysis. Using these differences, conditions in which G-quadruplex, a high-order structure, is stable were investigated.

Poster Presentation : **MAT.P-632**
Material Chemistry
Event Hall THU 11:00~13:00

Functionalization of zeolite for efficient mercury(II) adsorption

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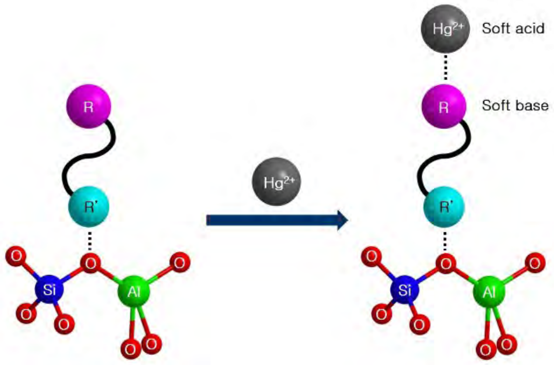
Mercury is highly toxic heavy metal that cannot be removed when it accumulates in the human body, resulting in symptoms such as paralysis and brain damage appearance. It is commonly encountered in daily life, and in particular, industrial processes are more open to experience to high concentration of mercury. Therefore, for mercury removal, there is an immense need for an effective method. According to the hard and soft acids and bases(HSAB) theory, mercury with soft acid properties can adsorb well to materials with soft base properties. This study is intended to effectively adsorb mercury by grafting a functional group with soft base properties in the zeolite. The ICP analysis results gave that after functionalization, more amount of mercury was adsorbed as compared with unfunctionalized zeolite. In addition, for optimization, numerous experiments were performed while changing either amount of grafting agent and/or time of catalyst synthesis, to obtain adsorbent for maximum adsorption of mercury.



Poster Presentation : **MAT.P-633**

Material Chemistry

Event Hall THU 11:00~13:00

A study on pre-oxidation of petroleum pitch-based activated carbons for electric double-layer capacitors

Jong Woo Kim, Soo-Jin Park*

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Electric double layer capacitors (EDLCs) are an excellent electrochemical energy storage system (ESS) because of their superior power density, faster charge–discharge ability, and longer cycle life compared to those of other EES systems. Activated carbons (ACs) have been mainly used as the electrode materials for EDLCs because of their high specific surface area, superior chemical sta-bility, and low cost. Petroleum pitch (PP) is a graphitizable carbon that is a promising precursor for ACs because of its high carbon content, which is obtained as an abundant by-product during the distillation of petroleum. However, the processibility of PP is poor because of its stable structure. In this study, pre-oxidized PP-derived AC (OPP-AC) was prepared to investigate the effects of pre-oxidation on the electrochemical behaviors of PP. The specific surface area and pore size dis-tribution of OPP-AC was lower and narrower, respectively, compared to the textural properties of untreated PP-derived AC (PP-AC). On the other hand, the specific capacitance of OPP-AC was 25% higher than that of PP-AC. These results revealed that pre-oxidation of PP induces a highly de-veloped micropore structure of ACs, resulting in improved electrochemical performance.

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Poster Presentation : **MAT.P-634**
Material Chemistry
Event Hall THU 11:00~13:00

Bicontinuous SiO¬2-CuxOy-TiO2 Heterostructure Prepared from Nanoporous Hybrid Fim (NHF) for Catalytic Applications

Kyeong Eun Yeo

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TiO2-supported catalyst has been in significant interest due to superior catalytic performance resulting from strong metal-support interaction (SMSI). However, the synthetic difficulty of porous TiO2 structure with high surface area and the insufficient stability of catalyst supported on TiO2 still impede extensive catalytic applications in many areas. In this context, bicontinuous SiO2-CuxOy-TiO2 heterostructure was prepared from nanoporous hybrid film (NHF) as a template. The high chemical and thermal stability of NHF enable to produce highly crystalline bicontinuous structure with high surface area. In addition, the core-shell-like bicontinuous urea/organosilica network directly provides porous silica-coated CuxOy-TiO2 structure by sequent impregnation of metal and metal oxide precursors and pyrolysis without post-deposition of silica layer. The porous silica coating layer not only enhances catalytic stability of the copper compound during catalytic reaction, but also leads to unique electronic structure at the interface compared to none-coated CuxOy-TiO2 structure. Furthermore, electronic structure of catalyst can be easily modified by changing organosilica precursor of NHF and impregnation sequence of metal and metal oxide precursors. Such different electronic structures at the interface greatly influence electron density and charge transfer rate between copper catalyst and TiO2 support, resulting in different catalytic activity and selectivity in catalysis. Here, we investigate how the structure and electronic structure of SiO2-CuxOy-TiO2 heterostructure at the interface affect catalytic stability and activity in photocatalytic synthesis of chemical compounds.

Poster Presentation : **MAT.P-635**
Material Chemistry
Event Hall THU 11:00~13:00

Synthesis of electroactive polyelectrolyte; containing carbazole and sulfonate moiety

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Carbazole based polymers have been developed over decades due to their photoconductive character and high hole transporting performance. Poly-(N-Vinyl carbazole) (PVK) can be synthesized by free radical polymerization method using free radical initiator such as 2,2'-Azobisisopropylnitrile (AIBN), thus, PVK was chosen as a base polymer to use for the development of p-type, anionic polyelectrolytes. In in this work, we synthesized a PVK polymer containing lithium sulfonate groups by co-polymerizing with the lithium allyl sulfonate (Li AS) monomer. By incorporation of the ionic Li AS unit, the hole transporting layer is able to self-dope, which allows it to function as a p-type interfacial layer in organic and hybrid semiconducting devices. Polymerization was carried out using a microwave reactor, and isolated using polar and non-polar solvents. Analysis by 1HNMR, FTIR and UV-vis analysis confirm the expected structure of the polymer. Future experiments will evaluate its effect on the electronic band structure of organic and perovskite solar cells, and its effect on device performance.

Poster Presentation : **MAT.P-636**
Material Chemistry
Event Hall THU 11:00~13:00

Electronic Alternation on BODIPY based Near-IR Dyes

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A series of BODIPY based near-IR dyes, **BODIPY TPA-H**, **BODIPY TPA-OMe**, and **BODIPY TPA-F**, was designed and prepared to study structural-property relationships depending on the peripheral group. Electrochemical- and photophysical properties of the developed BODIPY dyes were systematically investigated. All three compounds showed absorptions and emissions in the near-IR region. As attaching electron-donating substituents at the peripheral positions of the donor unit, the absorption showed a bathochromic shift with increased molar extinction coefficient value, while the emission quantum yield was decreased. On the other hand, both absorption and emission spectra showed a hypsochromic shift as attaching the electron-withdrawing group, and the quantum yield was increased. Finally, these compounds were applied to physiological temperature sensing from 77 K to 293 K, and **BODIPY TPA-OMe** showed the best sensing ability among the prepared compounds

Poster Presentation : **MAT.P-637**

Material Chemistry

Event Hall THU 11:00~13:00

The Role of the Bridging Unit on Triplet Excited State in Dyad System

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In this work, a series of carbazole–benzophenone based dyad compounds, **PCBP**, **XCBP**, and **PCTBP**, was designed and prepared to study the structure−property relationship depending on the bulkiness of the bridging unit. In the molecular design, the donor and acceptor units were linked by using different bridging units having different degrees of steric hindrance using benzene, xylene, and tetramethyl benzene rings for **PCBP**, **XCBP**, and **PCTBP**, respectively. Depending on the bulkiness of the bridging unit, they showed significantly different photophysical- and electrochemical properties, especially on their triplet excited states. Namely, when the donor and acceptor units were connected by benzene or xylene ring (**PCBP** and **XCBP**), they have electronic communications between the donor and acceptor units, which results typical charge transfer characteristics in the excited state. On the other hand, when the two units were connected by a tetramethyl benzene ring, **PCTBP**, electronic communications between the two units were almost perfectly isolated. In particular, the lowest triplet energy state (T_1) of the dyads were intriguingly affected by the bridging unit, thus T_1 state for **PCBP** and **XCBP** was generated at benzophenone unit while T_1 state **PCTBP** was generated at carbazole unit.

Poster Presentation : **MAT.P-638**

Material Chemistry

Event Hall THU 11:00~13:00

Applications of Multi-Wavelength Emission Luminophores for High-Efficiency Transparent Luminescent Solar Concentrators

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The Luminescent Solar Concentrator (LSC) is a device that produces electric energy by collecting sunlight as a waveguide employs luminescent dyes and concentrate the emitted energy on photovoltaic cells (Si PV cells) attached at the edges of the waveguide. The polymerizable inorganic cluster $[Re_6S_8(TBP)_4(VB)_2]$ is a promising candidate for LSC luminophores due to its broad photoluminescence at visible range. However, the low photoluminescent quantum yield (PLQY) and limited emission wavelength to the visible region of $[Re_6S_8(TBP)_4(VB)_2]$cannot significantly increase the performance of LSC. Here, we improved the performance of LSC by using ytterbium-doped $CsPbCl_3$ perovskite, which produces a PLQY of more than 100% by quantum cutting effect. This perovskite also has an emission wavelength in the near-infrared region, allowing us to utilize the 900-1200 nm region of Si PV cells, which could not be covered by $[Re_6S_8(TBP)_4(VB)_2]$ alone. The synthesized dyes were uniformly applied to the polymer matrix and fabricated into LSC and used for various performance measurements. Our chemically/physically stable LSC suggests a practical future direction for smart windows.

Poster Presentation : **MAT.P-639**

Material Chemistry

Event Hall THU 11:00~13:00

Tunable optical and electrical properties of sputtered tin-doped indium oxide thin films grown in oxygen free atmosphere

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Tin-doped indium oxide (commonly named as ITO) is a well-known material vastly used due to its unique behavior of high transparency with electrically low resistive properties. Sputtering is the most common technique due to its large scale, uniform, controllable thin film fabrication approach. To grow high quality sputtered ITO thin films, parameters such as sputtering pressure, power, substrate temperature and dopant concentration plays a key role for its application as transparent electrodes [1-5]. In this work, we have demonstrated the holistic control of optical and electrical properties of sputtered ITO thin films deposited on glass substrates under different process conditions of sputtering pressure, power, and substrate temperature in oxygen free atmosphere. The indium–tin alloy sputter target is used with fixed weight proportion (In2O3:SnO2::9:1). To achieve the process optimization window and to understand the correlation with sputtered ITO films, we have used various characterization techniques including XRD to understand structural behavior, UV-vis spectroscopy for the transmittance as well as reflectance behavior and room temperature Hall measurement to obtain key electrical parameters of resistivity, mobility and carrier concentration. The optimized condition for highly transparent and conductive ITO films on glass substrate is observed with RF power ~ 200 W, working pressure ~ 3.5 mTorr and at the substrate temperature of 400 °C. The corresponding optimum values are; transmittance ~ 97% (in visible region), sheet resistance ~ 10.6 Ω/□, resistivity ~ 1.62 × 10-4 Ω.cm, mobility ~ 39.5 cm2/V-s, carrier concentration ~ 9.77 × 1020 cm-3. These performance characteristics of sputtered ITO films can be used for transparent electrode in various device applications.

Poster Presentation : **MAT.P-640**

Material Chemistry

Event Hall THU 11:00~13:00

Hafnium Nitrides with Nitrogen Defects and Their Magnetic Properties

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Hafnium nitride (HfN) typically crystallizes in the cubic rock-salt structure and are widely used in electronic materials due to its unique chemical and physical properties. We report on the solid-state synthesis of hafnium nitrides with the nitrogen defects and their magnetic properties. Synthesis experiments were performed using HfNCl and NaN_3 as precursors in an evacuated quartz tube. HfNCl adopts the layered structure, which consists of double honeycomb HfN layers intervened by chloride ions. The resulting HfN materials were fully characterized by X-ray diffraction, thermogravimetric analysis, scanning electron microscopy, and a SQUID magnetometer. Synthetic methods and the effect of nitrogen-deficiency on superconducting properties are described in detail.

Poster Presentation : **MAT.P-641**

Material Chemistry

Event Hall THU 11:00~13:00

A fast and simple method for fabricating superhydrophobic surface via solution spray-coating at room temperature

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Department of Chemistry, Kyonggi University, Korea

It is a widely known fact that superhydrophobic properties have been discovered in nature and studied as a biomimetic technology to apply them to real industries. Many researchers have recently studied to make superhydrophobic surfaces (SHS) through simple and inexpensive methods. This research used a two-stage coating method to manufacture SHS quickly and simply in a solution process. First, by spraying the metal precursor solution, a rough surface of metal oxide could be obtained, then the roughness could be improved while reducing surface free energy by spraying the solution of alkylphosphonic acid. The manufactured SHS exhibited a high water contact angle (WCA) above 150 ° and showed a sliding angle (SA) of about 10 °. The method introduced in this study can be applied to various substrates such as silicon wafers, glass, metal, and synthetic fibers, and is expected to be easily used in fields requiring waterproofing in the future.

Poster Presentation : **MAT.P-642**

Material Chemistry

Event Hall THU 11:00~13:00

Enhancement of Thermoelectric Properties by Exchange Interaction with Localized Magnetic Impurities and Itinerant Electrons

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Thermoelectric materials have attracted considerable research attention in recent years due to their ability of reversible conversion between heat and electricity. The enhancement of thermoelectric performance is challenging due to the strong correlation of Electrical conductivity and Seebeck coefficient. In this work, we studied eco-friendly Cr-doped Cu_2SnS_3 nanocomposite with $CuCrSnS_4$. Our experiments and theoretical calculation(DFT) proved that doping the Cr atom in Sn site of Cu_2SnS_3 enhanced electrical conductivity by modifying the density of state of electrons. Moreover, by DFT calculation, it is found that doping Cr atom in Sn site makes the chemical bonding soften resulting in lattice thermal conductivity decrease. Using XRD analysis, the solubility limit of Cr impurity in Cu_2SnS_3 is around 5 at%. Doping Cr atom above the solubility limit induced the spinel $CuCrSnS_4$ nanoprecipitations. The superparamagnetic fluctuation of spin angular momentum of spinel $CuCrSnS_4$ results in exchange interaction with itinerant carrier spin. The synergetic effect of Cr doping made the power factor increase from 1.12 to 6.67 $\mu W/cm/K^2$. The $CuCrSnS_4$ were verified that second phase in Cu_2SnS_3 matrix by XRD and TEM analysis. Finally, Cr-doped-Cu_2SnS_3 with magnetic nanoparticles showed the highest average zT value of 0.8 at 723 K comparing with pristine zT of 0.08 at 723 K.

Poster Presentation : **MAT.P-643**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and Photophysical Properties of Light-Harvesting Gold Nanoclusters Fully Functionalized with Antenna Chromophores

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The development of efficient light-harvesting systems is critical to understand the key aspects of solar-energy conversion processes and to utilize them in various photonic applications. Here, atomically well-defined gold nanoclusters were synthesized as a new platform to mimic light-harvesting systems. An efficient amide coupling method is developed to synthesize water-soluble Au_{22} clusters with densely packed 18 pyrene chromophores (Au_{22}–PyB_{18}) by taking advantage of their facile phase-transfer reaction. A combination of femtosecond transient absorption and anisotropy measurements provided a clear picture of energy transfer/migration processes occurring in Au_{22}–PyB_{18}. Consequently, the photoluminescence of Au_{22} is enhanced by more than 10-fold, demonstrating that pyrenes at the periphery efficiently channel the absorbed energy to the luminescent Au_{22} at the center. Moreover, the synthesized Au_{22}–PyB_{18} led to unique triple-emission in blue, green, and red wavelength regions arising respectively from pyrene monomer, excimer, and Au_{22} emission, generating bright white light emission together. The structurally well-defined gold clusters exhibiting unique luminescent properties constitute a powerful model system to gain deeper understanding of the solar energy conversion processes. Further, the newly developed conjugation method for the preparation of highly functionalized gold clusters may have broad implications not only in photonic applications but also in other biological areas.

Poster Presentation : **MAT.P-644**
Material Chemistry
Event Hall THU 11:00~13:00

Orientation Change of Electrospun Nanofibers by Collector Design

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Department of Chemistry, Hanyang University, Korea

Electrospinning is a technology that can fabricate fibers with uniform diameters in nanoscale. These fibers can be used for tissue engineering by mimicking ECM in vivo. It is also attracting attention in many areas such as filters and electronics by utilizing the versatile physical and chemical properties of fiber substrates. However, it is not easy to form a substrate of a desired shape by arranging fibers using electrospinning, and it still remains a challenge. Therefore, in electrospinning, since the collector where fibers are deposited is greatly affected, many studies are being conducted to change the shape of the collector to control the fiber arrangement and change the arrangement of fibers or the amount of deposition.In this study, we designed several flat aluminum collectors with holes. Here, the tendency of PCL nanofiber deposition, which is formed by changing the size, shape and number of holes, and the shape of the collector as parameters, was studied together with an electric field. Also, in order to analyze the cause of this trend, simulation was performed using COMSOL, and the orientation of the fiber was checked through ImageJ.

Poster Presentation : **MAT.P-645**

Material Chemistry

Event Hall THU 11:00~13:00

High Resolution Nano-scale Patterning Performed by Atomic Force Microscopy Lithography

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Atomic Force Microscopy (AFM) Lithography can precisely perform specific patterning at nano-scale locations and create nano-structures confined to specific areas due to imaging functions. This technology can induce various physical and chemical processes on the surface of the substrate based on the interaction between the probe and the substrate. It can be classified into two main categories. i) Contact Lithography ii) Non-Contact Lithography. Contact Lithography is a method that uses the interaction between the tip and substrate by applying a large force to the tip to make a pattern. Non-Contact Lithography is a method of making patterns by forming an oxide layer by adjusting tip bias. In this study, we designing patterned using Contact Lithography and Non-Contact Lithography methods on a silicon substrate using nano-scale tips. By changing the drawing speed of the tip and the force applied, precise patterning is performed to identify the tendency and control it to the desired size. This is a technology that will be widely applied in various aspects in the future.

Poster Presentation : **MAT.P-646**
Material Chemistry
Event Hall THU 11:00~13:00

Post functionalization of organic agents in zeolite micropore for olefin/paraffin separation

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Being major feedstock for petrochemical industry, light olefins such as ethylene and propylene are obtained by the steam cracking of naphtha. Due to similar physical properties, the separation of olefin and paraffin is the key processes to meet the olefin purity requirements. Generally, energy-intensive cryogenic distillation process is used at low temperatures and high pressures. Apart from that, adsorption using suitable adsorbents is an alternative process that is cost-effective and consume low energy for olefin/paraffin separation. This study is focused on separation of light olefins using post-functionalized MOR zeolite. Numerous organic functionalizing agents (i.e., benzene, fluorobenzene, aniline and etcs.) were grafted on MOR zeolite micropores . By controlling the zeolite micropore size through post-functionalization, can help in selective adsorption of olefins. Change in the physicochemical properties of functionalized zeolite was confirmed using varipous isotherm techniques. The adsorption selectivty of each adsrobent was caculated following IAST equation. A significant change in selectivity for olefin was observed.

Poster Presentation : **MAT.P-647**

Material Chemistry

Event Hall THU 11:00~13:00

Tunnel β-$Ca_{0.17}V_2O_5$, Calcium Bronze Vanadate as a Cathode Material for Ca-Ion Batteries

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Small rods of β-$Ca_{0.17}V_2O_5$, a calcium bronze vanadate has been studied for the first time as cathode material for calcium-ion batteries (CIBs). It has tunnel structure which allowing calcium insertion and extraction into the host material. The intercalation mechanism has never been reported in other ion batteries system. Herein, we demonstrate of β-Ca0.17V2O5 as the cathode material for CIBs. It shows reversible capacity 130 mAh g^{-1} at 10 mA g^{-1} at 25 °C in $Ca(BF_4)_2$ in EC:PC with an average voltage around 3.12 V (vs. Ca/Ca^{2+}). Even though, it shows not much structure changes, a reversible X-Ray diffraction evolution during discharge-charge reveal the feasibility calcium intercalation. This research brings more knowledge to investigate calcium ion intercalation chemistry into host material.

Poster Presentation : **MAT.P-648**

Material Chemistry

Event Hall THU 11:00~13:00

Fabrication of a facile and robust superhydrophobic surface using functional-POSS

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Inspired by nature, superhydrophobic surfaces, which have a water contact angle (WCA) greater than 150° and a small sliding angle (SA), have attracted great interest for their several properties. Therefore, superhydrophobic coatings can be applied to self-cleaning, anti-icing, oil-water separation, etc.In this experiment, we synthesized functional POSS(F-POSS) with the optimized ratio of UV crossable vinyl groups for film networking and octadecyl groups for hydrophobicity via thiol-ene click reaction between Vinyl-POSS (polyhedral oligomeric silsesquioxanes) and octadecanethiol under UV irradiation at room temperature. Moreover, by adding a cross-linker(dithiol), we can fabricate a stable hybrid superhydrophobic surface under UV irradiation by facile solution spray coating. The coated surface resulted in a contact angle greater than 150° and to verify the durability of the coated surface several tests were performed, also, F-POSS coatings can be fabricated onto various substrates.

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Poster Presentation : **MAT.P-649**

Material Chemistry

Event Hall THU 11:00~13:00

Solid solutions of delafossite-phase $CuCrO_2$ and $CuGaO_2$ for application to hole conductor of perovskite solar cells

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$CuCrO_2$ (CCO) and $CuGaO_2$ (CGO) with delafossite 2D crystal structures have often been used as hole-transporting materials (HTMs) for p-i-n type perovskite solar cells. CGO synthesized by hydrothermal reaction has a hexagonal disk-like structure with high crystallinity with a size of 100 nm or larger. Because of its large particle size, CGO is not suitable for forming uniform films on the top of the highly rough FTO or ITO surfaces. On the other hand, hole-conducting property of CCO is relatively inferior to that of CGO, but uniform nanoparticles (NPs) of CCO can be obtained by a simple hydrothermal reaction. Therefore, in this study, $CuCr_{1-x}Ga_xO_2$ (CCGO) NPs of various compositions were synthesized to obtain the advantages of CCO and CGO. The prepared CCGO NPs were then applied as HTMs of p-i-n type PSC devices using $MAPbI_3$ as a light absorber, and CCGO with a Ga content of 60% showed the best PV characteristics. The achieved photovoltaic conversion efficiency (PCE) was over 16%, which is much higher than that of PSCs with bare CCO or CGO.

Poster Presentation : **MAT.P-650**

Material Chemistry

Event Hall THU 11:00~13:00

A Novel Approach of Layered Molybdenum Oxides Exfoliation : Collapse of Interlayer Interaction by Au Nanoparticles Growth

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Two-dimensional layered materials can be applied in various fields due to their unique optical properties, mechanical strength, and electrical conductivity. For those potential applications , it is important that the two-dimensional materials should be prepared consistently with a thin layer. Therefore, various methods have been developed such as electrochemical and mechanical exfoliation to make homogeneous substances. Although these methods have exhibited many advantages, it has crucial weaknesses in terms of surface stability and thickness uniformity . In this study, we suppose to suggest a new exfoliation method to overcome the disadvantages of previous studies. The new idea we proposed is breaking the interlayer forces, which maintain layered structures. We employed layered MoO_3 as a host material, and Au ions were used as a source of nanoparticles to produce hybrid structures. Through the intercalation of gold ions between the interlayer space of MoO_3 and the growth of Au NPs on the layer, the interlayer forces of MoO_3 become weakened, and finally, we were able to obtain the $Au@MoO_3$ hybrid structure . The $Au@MoO_3$ hybrid nanostructure was characterized by UV-Vis spectrophotometer, XRD, and TEM. Through these analyzes, we confirmed the presence of Au NPs on MoO_3 with a thinner layer.

Poster Presentation : **MAT.P-651**

Material Chemistry

Event Hall THU 11:00~13:00

Selective Photooxidation of Lignin Derivatives by Plasmonic Au Nanocatalysts under Visible Light Illumination

Jiwon Kang, Youngsoo Kim[1,*]

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[1]*Department of Chemistry, Yeungnam University, Korea*

Researchers have been made an effort to develop a sustainable energy source as an alternative to fossil fuels, which are major cause of global warming. Lignin is a massive natural polymeric material composed of aromatic compounds and its derivatives, and have been recognized as a suitable materials that can substitute of petrochemicals. Because of the huge molecular structure of natural lignin, it is difficult to utilize in many industrial fields, hence, it is important to be split into a simple aromatic compound which is small molecule to easy use. Decomposition techniques of natural lignin have been developed such as chemical treatment, physical treatment, and biological treatment methods. However, these techniques cause severe problems that require harsh reaction conditions or generate harmful chemicals while decomposition process. Photocatalytic lignin conversion is one of the most promising technique because it is eco-friendly and less energy consumption. In this study, we demonstrated photocatalytic lignin degradation using plasmonic Au nanocatalysts and the monochromatic visible light source. And we conducted experiments to reveal mechanistic insight of lignin degradation. We characterized the resultants through various analytical tools like optical spectroscopy, chromatography, and NMR. As a results, we found that the lignin model compound was selectively oxidized by plasmonic Au nanocatalysts rather cleavage of chemical bonds.

Poster Presentation : **MAT.P-652**

Material Chemistry

Event Hall THU 11:00~13:00

Fe-NiSe/NF as a High Performance Electrocatalyst for Oxygen Evolution Reaction

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Renewable and green energy sources have received widespread attention due to global interests in decreasing CO2 emission. Developing low-cost and stable electrocatalysts with high activity for oxygen evolution reaction (OER) is important issue to realize cost-economic hydrogen production using electrolysis of water. Because of sluggish kinetics of OER processes, most reported OER catalysts based on transition metals exhibit high overpotential. To overcome this issue, we use transition metal chalcogenide as an electrocatalyst which exhibit outstanding electrochemical performance. Fe-NiSe is synthesized on Ni foam through simple two-step hydrothermal synthesis process. Fe-NiSe deposited on a Ni foam (designated as Fe-NiSe/NF) exhibits low overpotential of 204 mV at 10 mA cm-2 and Tafel slope of 42.6 mV dec-1 in 1 M KOH solution. In addition, chronopotentiometry shows that Fe-NiSe/NF is stable over 100 hours in alkaline solution.

Poster Presentation : **MAT.P-653**

Material Chemistry

Event Hall THU 11:00~13:00

Enhanced Oxygen Evolution Reaction Performance of Ba0.5Sr0.5Co0.8Fe0.2O3-δ Perovskite with Induced Dipole

HongDeok Park, Jae Ryeol Jeong, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Polarization of ferroelectric materials can accelerate electron transfer, leading to the enhanced electrochemical catalytic property. By a high-voltage poling process, polarization domains of ferroelectric materials can be aligned in the desired direction. In this work, we synthesized 〖Ba〗_0.5 〖Sr〗_0.5 〖Co〗_0.8 〖Fe〗_0.2 O_(3-δ)(BSCF), perovskite oxides with high oxygen evolution reaction (OER) efficiency, and polarized sample by a poling process. XPS and electrochemical active surface area (ECSA) proved that positively poled samples show an increase of surface (+) charge, which makes improved 〖OH〗^- adsorption. Therefore, these samples display enhanced electrochemical performance for OER. This study proposes a new improvement strategy using established high performance ferroelectric material-based electrocatalysts.

Poster Presentation : **MAT.P-654**

Material Chemistry

Event Hall THU 11:00~13:00

Enhanced Electrochemical Performance of Hybrid MOF Structure

Hye Yeon Yoo, Min Hyung Lee[1,*]

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[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Interest in hydrogen as an alternative energy source is increasing, but current hydrogen production relies on a gas reforming processes which uses fossil fuels and causes environmental problems. Therefore, it is essential to develop eco-friendly hydrogen production methods, and electrochemical water electrolysis is considered one of those. The oxygen evolution reaction (OER) is the half-reaction of hydrogen production via water splitting. However, the OER requires a higher over potential compared to the hydrogen evolution reaction (HER), so OER is the most challenging huddle for realizing the commercialization level of hydrogen production through water electrolysis. The Metal-Organic Frameworks (MOF) is a material with a large surface area due to its unique structure and has been applied to various catalyst studies. In this poster, a hybrid structure was synthesized using two MOFs. The synthesized hybrid structure MOF catalyst showed improved electrochemical catalytic performances.

Poster Presentation : **MAT.P-655**

Material Chemistry

Event Hall THU 11:00~13:00

Ni-Fe/ZIF-67 Composites for a Promising Electrocatalytic Oxygen Evolution Reaction

Da Kyoung Jung, Min Hyung Lee[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

As recent environmental issues due to global warming gas emission, interests in green and sustainable energy technologies are attractive. Among various alternative energy sources, hydrogen energy gets spotlight due to its high energy density without CO2 emission. Unfortunately, sluggish reaction kinetics of oxygen evolution reaction (OER) at the anode is a major source of low efficiency of hydrogen production in water electrolysis. Therefore, it is essential to exploit low-cost, high-efficient, and non-noble metal catalyst for OER to reach hydrogen production in industrial level. Hence, in this work, we synthesized ion-exchanged trimetallic catalyst of Ni-Fe/ZIF-67 by a simple solution process at the room temperature. Synthesized Ni-Fe/ZIF-67 catalysts show excellent electrochemical performance for OER with an overpotential of 220 mV and stability over 20 h without noticeable changes at current density of 10 mA/cm2.

Poster Presentation : **MAT.P-656**

Material Chemistry

Event Hall THU 11:00~13:00

Novel Electrochemical Catalysts: Organo-Metallic Complex Inserted Montmorillonites

In Seon Lee, Jae Ryeol Jeong[1], Min Hyung Lee[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1] *Department of Applied Chemistry, Kyung Hee University, Korea*

Recently, researches on developing sustainable and highly efficient energy that can overcome global warming issue have been attracting great attention. Green hydrogen energy production using water electrolysis have been heavily studied due to its potential as a sustainable and clean energy production. However, it is still difficult to achieve industrial level production of hydrogen due to the sluggish process of four-electron transfer process of oxygen evolution reaction (OER). Therefore, electrocatalysts wih high electrochemical performance are required to reduce the overpotential for water oxidation. In this study, we focus on montmorillonite (MMT) clay material, which has layered structure where ogrgano-metallic compelex can be inserted in the interlayer under host-guest reaction. Organo-metallic complex inserted MMTs exhibits decreased overpotential in the order of Co>Ni>Fe at 10 mA/cm2.

Poster Presentation : **MAT.P-657**

Material Chemistry

Event Hall THU 11:00~13:00

The Effect of Iron on Enhancing Oxygen Evolution Reaction Performance of Manganese Oxide

Cu Dang van, Min Hyung Lee[1,*]

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[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

The oxygen evolution reaction (OER) has been an important part of many energy conversion and storage devices such as fuel cell, metal-air batteries, CO2 reduction cell. Recently, manganese oxide, earth-abundant oxygen catalysts, is attracting to develop as OER catalyst thanks to its low cost, natural abundancy, environmental friendliness and well-balanced activity-stability performance. However, a large overpotential is still required to reach a current density of 10 mA cm-2 in alkaline electrolyte. Herein, we applied a simple method to synthesize Fe-doped MnO2 (Fe-MnO2) on Ni foam for OER electrode. Compared to the pristine MnO2 (the overpotentials of 622 and 758 mV at 100 and 1000 mA cm-2, respectively), Fe-MnO2 shows the huge enhancement of OER activity with the overpotentials of 304 and 379 mV at 100 and 1000 mA cm-2 in 1 M KOH electrolyte, respectively. Moreover, Fe-MnO2 exhibits the excellent stability at the current density of 300 mA cm-2 for 12 hours without noticeble degradation.

Poster Presentation : **MAT.P-658**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis and Characterization of D-A-D' Type Random Copolymer as organic solar cell Donor Polymers

Ji Hyun Lee, Yun Hi Kim[1,*]

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[1]*Department of Chemistry, Gyeongsang National University, Korea*

We synthesized a D-A-D' type random copolymer series, that are based on poly[(2,6-(4,8-bis(5-(2-thioethylhexyl-3-chloro)thiophen-2-yl)benzo[1,2-b:4,5-b′]dithiophene))-alt-(5,5-(1′,3′-di-2-thienyl-5′,7′-bis(2-ethylhexyl)benzo[1′,2′-c:4′,5′-c′]dithiophene-4,8-dione)] (PBDB-S-3Cl) and poly[(2,6-(4,8-bis(5-(2-thioethylhexyl-4-chloro)thiophen-2-yl)benzo[1,2-b:4,5-b′]dithiophene))-alt-(5,5-(1′,3′-di-2-thienyl-5′,7′-bis(2-ethylhexyl)benzo[1′,2′-c:4′,5′-c′]dithiophene-4,8-dione)] (PBDB-S-4Cl), PBDB-S-CO-3Cl-4Cl (1:9), PBDB-S-CO-3Cl-4Cl (3:7) PBDB-S-CO-3Cl-4Cl (7:3) and PBDB-S-CO-3Cl-4Cl (9:1) for the research of the effects of substitution position of chlorine of PBDB-S on its solar performance. The composition modulation of random copolymers with the effects of substitution position of chlorine affect the organic solar cell performance. The PBDB-S-CO-3Cl-4Cl (9:1) random copolymer shows the highest FF of 0.63 and PCE of 13.31 %, which performance was higher than those of homopolymer PBDB-S-4Cl and PBDB-S-3Cl.

Poster Presentation : **MAT.P-659**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation of Porphyrin Aggregate Contained Polyurea Network coated TiO2 for High H2O2 Production

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[1]*School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea*

Porphyrin aggregates are promising materials for mixing with TiO2 owing to their high light adsorptivity and charge separation efficiency. Porphyrin aggregate has been made either by the self-assembly of porphyrin molecules or by the preparation of porphyrin-based framework particles. However, the conventional method is difficult to evenly form a stable porphyrin aggregation layer on TiO2. Here, we show that controlled porphyrin aggregates can be uniformly and stably coated on TiO2 using a porphyrin-based polyurea network (PN) nanogel. The PN nanogel is made by mixing tetrakis(4-aminophenyl)porphyrin (TAPP) and hexamethylene diisocyanate (HDI) which is the same as the organic sol-gel method. The nanogel was applied to the TiO2 surface by using a spin coating method to yield a PN coated TiO2 (PNT). The several nanometer nanogel layers uniformly coated TiO2 nanoparticles. The rearrangement reaction of PN by thermal treatment of PNT produced a rearranged PN (RPN) coated TiO2 (RPNT). UV-Vis analysis confirmed that porphyrins form J-aggregates in the PN and RPN layer. Both layers have a short photoluminescence lifetime, indicating their high charge separation efficiency. Although PNT and RPNT show high photocatalytic H2O2 production, RPNT show higher H2O2 production thanks to its high surface area.

Poster Presentation : **MAT.P-660**

Material Chemistry

Event Hall THU 11:00~13:00

Fabrication of Controllable Hydrogel-Based Hollow Structure by using Hybrid Technique for Future Artificial Organ

Yeeun Cho, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Fabrication of hollow structures such as blood vessels, the heart, stomach, bladder, or intestine, which comprise our body, received enormous concern in tissue engineering development. Tissue engineering strategies to mimic the native tissue construct and organs pose an opportunity and great challenge. We develop a novel strategy to fabricate the hollow structure, mimicking the hollow structure of the hollow organs using the hybrid fabrication system. In particular, we designed a diffusive technique by incorporating calcium chloride in Pluronic F127 (PF127-Ca) as a fugitive ink and subsequently casting alginate and gelatin mixture over the extruded PF127-Ca. After extruding PF127-Ca on the top of the alginate-gelatin mixture, calcium ions will diffuse, crosslink the alginate, and yield a hollow hydrogel construct that physically mimics the hollow organs. The properties of the vessel can be controlled by changing the CaCl2 concentration, diffusion time, and nozzle size during the printing process. The fabricated hollow structure, mimicking the native organs, provides a potential platform to study artificial organs to replace or understand the organism's digestive system.

Poster Presentation : **MAT.P-661**

Material Chemistry

Event Hall THU 11:00~13:00

Sputter-deposited metal oxide thin films for application to perovskite solar cells

Woo seok Suh, Wan-In Lee[1,*], Songhyeon Jung, Park Geonho

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[1]*Department of Chemistry, Inha University, Korea*

Oxide semiconductors such as TiO2 and SnO2 which have excellent chemical stability and high electron mobility have been extensively investigated as electron transporting material (ETM) for perovskite solar cells (PSCs). In the present study, we prepared compact TiO2 and SnO2 layers by sputtering process and compared the electron-transporting properties of these two materials. When they were applied as the ETM of n-i-p type PSC devices employing FAPbI3 as light absorber and spiro-OMeTAD as hole transport layer, it was found that SnO2 leads to relatively higher power conversion efficiency (PCE). We also varied the thickness of TiO2 and SnO2 layers to determine the optimal thickness for the electron transport. In particular, when the thickness of SnO2 layer was 30 nm, the fabricated solar cell device exhibited a PCE of 21.59% at VOC of 1.059 V, JSC of 25.73 mA/cm2, and FF of 79.28%. We analyzed the thin film structures deposited on the highly rough FTO substrate and discussed the reason for the higher PV performance of SnO2-based PSC devices.

Poster Presentation : **MAT.P-662**

Material Chemistry

Event Hall THU 11:00~13:00

Sustainable development of a multifunctional porous carbon for CO_2 Capture

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[1]*Gyeongnam National University of Science and Technology, Korea*
[2]*Ulsan National Institute of Science and Technology, Korea*
[3]*Department of Energy Engineering, Gyeongsang National University, Korea*

The climatic concerns aroused from the energy produced via fossil fuel require the solution for emitted CO_2. The solid porous adsorbents are conceived as the potential alternative for the liquid amine solution due to their robust stability and lower energy penalty for regeneration. Herein, a hetero-atom functionalized high surface area porous carbon derived from a low surface area porous polymer using an environmentally friendly method is studied for CO_2 capture. Traditionally, KOH is used to produce activated carbon but its corrosive nature has presented several challenges to make the activated carbon at a large scale. Herein, we have used potassium oxalate as an activator. Interestingly, the yield of carbon using potassium oxalate is more than KOH, and it is not toxic. The sample activated at 800 °C possessed high SABET of 2302 m^2/g. The micropores in conjunction with hetero atom boost the capture efficiency of the adsorbents. Upon the subjecting, to CO_2 capture application, a capture capacity of 17.2 mmol/g at 25 bar and 298 K was observed. Interestingly, the heat of adsorption estimated using the Clausius Clapeyron equation was calculated to be 25.2 kJ/mol, indicating that the interaction of CO_2 with the adsorbents is physisorption in nature, and regeneration can be made using pressure swing adsorption method or by normal heating, as the physical forces in comparison to chemical forces are week. The IAST selectivity with gas composition 15:85 CO_2 vs. N_2 (similar to flue gas) was found to be 13 at RT. These observations make the developed carbon a suitable adsorbent for CO_2 capture.

Poster Presentation : **MAT.P-663**

Material Chemistry

Event Hall THU 11:00~13:00

Supramolecular nanomachine via molecular folding and unfolding

Soyeong Jin, Jaegeun Noh[1,*], Youngdo Jeong[2,*]

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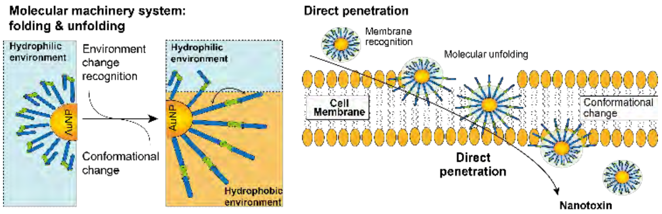
[2]*Biomedical Research Institute, Korea Institute of Science and Technology, Korea*

As biological nanomachines, proteins and nucleic acids can activate their function through conformational change induced by supramolecular recognition in living processes. Although the use of synthetic nanomachines that mimic biological functions for therapeutics is promising, the development of artificial nanomachines for therapeutics is still restricted to the lower hierarchical level of the molecular components. Herein, we present an artificial nanomachine in which actuatable molecular machines are integrated into a hierarchical nanomaterial in response to external stimuli to regulate biological functions. Protein-sized gold nanoparticles are covered with ligand layers as machinery parts, whose folding/unfolding locomotion response to the cellular environment allows the direct penetration of the nanoparticles across the cellular membrane to disrupt intracellular organelles. Additionally, the pH-responsive latch molecules as a switch can control the conformational changes of the molecular machines, inducing the selective apoptosis of cancer cells. This approach based on the mechanical motion of molecular components on a hierarchical nanocluster would be an effective platform for biomimetic nanomachines.



Poster Presentation : **MAT.P-664**

Material Chemistry

Event Hall THU 11:00~13:00

Chemiresistive gas sensor based on light promoted-COF film

Seungcheol Kim, **Hyunseob Lim**[1,*]

Chemistry, Gwangju Institute of Science and Technology, Korea

[1]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

Covalent organic framework (COF) has been widely investigated for a variety of applications such as gas storage, catalysis, and sensor due to its high surface area, crystalline porous structure, modifiable functionality, and stability. Generally, to synthesize the COF, solvothermal method which utilizes thermal energy to form crystalline COF has been usually used. However, this method requires very long time and gives insoluble powder form. Long time consuming is not proper in perspective of efficiency and this insoluble COF powder is difficult to process, which makes difficult to fabricate device. Thus, we have introduced light source to synthesize COF highly fast and liquid-air interface which is a 2D-confined platform for 2D COF film. Herein, we synthesized imine based COF film on the water surface using Xe lamp and fabricated chemiresistive gas sensor device. 1,3,5-Tris(4-aminophenyl)-benzene (TAPB) and terephthaldehyde (PDA) were used to form imine based COF in which nitrogen atom may be adsorption site for some gas molecules having possibility for hydrogen bonding. We have been guessing hydrogen bonding based interaction make intramolecular charge transfer possible.

Poster Presentation : **MAT.P-665**

Material Chemistry

Event Hall THU 11:00~13:00

Selective functionalization of monolayer h-BN with diazonium salt via electrochemical reaction for generating midgap energy states

Younghee Park, Hyunseob Lim[*]

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We demonstrated the new chemical route to facilitate the direct functionalization on insulator, h-BN. Aryl groups were successfully functionalized on the h-BN by the electrochemical reduction reaction of 4-BBDT. Although many efforts have been made to functionalize the surface of h-BN, it has been reported that general spontaneous reactions rarely occur. Because h-BN is an insulator, having large band gap (~6 eV), single electron transfer from h-BN to organic precursor is difficult, which is regarded as prerequisite process for radical-based functionalization reactions. The electrochemical process can drive the electron tunneling from working electrode to 4-BBDT through h-BN film (both monolayer and multilayer) by electron tunneling process, and produce the highly reactive diazonium radical on its surface. Then, aryl radicals can be covalently functionalized on h-BN surface. In addition, this rapid reaction process can modulate the electronic structure of h-BN. We believe that our demonstration does not only provide fundamental insights for developing the surface functionalization reaction on 2D materials, but also can advance the applications of h-BN-based optoelectric devices.

Poster Presentation : **MAT.P-666**

Material Chemistry

Event Hall THU 11:00~13:00

Growth of Tungsten disulfide Monolayer Using Vapor Pressure-Controllable Molecular Inorganic Precursor

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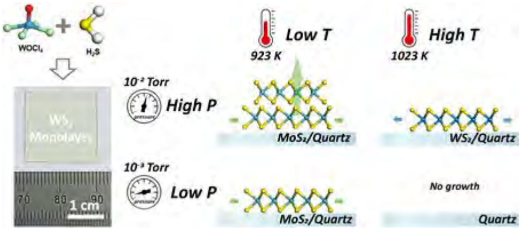
Among the two-dimensional (2D) transition-metal dichalcogenides (TMDs), MoS2 receives considerable attention, but WS2 is also a good representative TMD material because of its unique physical properties, such as having the relatively high electron mobility of 400 cm2V-1s-1 theoretically, and a large valence band splitting caused by strong spin-orbit coupling and strong photoluminescence (PL). In particular, outstanding properties, such as a large bandgap of 2.02 eV and strong PL caused by direct bandgap, appear in the monolayer. These outstanding characteristics have attracted considerable interest in the large-area and homogeneous growth of WS2 monolayers with good quality. Significant effort has been reported using several kinds of chemical vapor deposition (CVD) methods to improve the growth process for monolayer WS2, especially to achieve high crystallinity and homogeneity. Herein, we demonstrate the large-scale growth of high-quality monolayer WS2 film with outstanding homogeneity using WOCl4 and H2S by an inorganic vapor CVD (IVCVD) system. The carbon-free elemental composition of WOCl4 prevented carbon contamination effectively during the growth process, which is confirmed using Raman spectroscopy, and the growth rate was significantly improved by several tens of minutes. A significant part of the growth mechanism of 2D TMD materials using the CVD method is still unknown, despite its technological advancement. My comparative study with respect to MoS2 on the properties of molecular precursors and the thermodynamics of the growth reaction could extend the understanding of growth mechanisms. The optimized reaction conditions based on a systematic investigation of the effect of growth parameters facilitated the termination of WS2 growth at the monolayer.


WOCl₄
H₂S
WS₂ Monolayer
70
80
90
1 cm
10⁻² Torr
High P
10⁻³ Torr
Low P
Low T
923 K
High T
1023 K
MoS₂/Quartz
WS₂/Quartz
MoS₂/Quartz
No growth
Quartz

Poster Presentation : **MAT.P-667**

Material Chemistry

Event Hall THU 11:00~13:00

RuO$_2$ Supported on the PdPb Nanosponges Show Enhanced Electrocatalytic Activity and Stability for OER in acidic media

Doyeop Kim, Kwangyeol Lee*

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Hydrogen production through electrochemical water splitting is potentially carbon-free, and can be a primary pathway to reduce fossil fuel usage. The sluggish kinetics of oxygen evolution reaction (OER) half-reaction is a key hurdle to overcome in boosting the reaction efficiency. Although Ru-based nanocatalysts exhibit excellent activities for the acidic OER, they are prone to be dissolved in acidic conditions. Herein, we synthesized RuO$_2$ on the PdPb nanosponge via seed-mediated growth and subsequent thermal oxidation to stabilize the Ru-based nanocatalyst. The prepared RuO$_2$ on the PdPb nanosponges exhibited excellent catalytic activity and stability in acidic OER.

Poster Presentation : **MAT.P-668**

Material Chemistry

Event Hall THU 11:00~13:00

Synthesis of Au-Cu_2O Heterostructures as Nanocatalysts for the Electrochemical CO_2 Reduction into C_{2+} Products

Minah Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

With the ever-growing concerns for pollution and climate change today, necessary steps must be taken to reduce the abundant amount of carbon dioxide in the air and put it into efficient use. Carbon dioxide reduction reaction (CO_2RR) has been the key to this issue, where it can produce various essential fuels and feedstocks such as carbon monoxide, methane, methanol, formate, ethylene, and ethanol. However, since carbon dioxide exists as a thermodynamically stable compound, highly active catalysts are required for this electrochemical reaction. Moreover, most attention is leaned towards the production of catalysts capable of producing high-value C_{2+} products with high selectivity. Herein, we report the synthesis of Au@Cu_2O hetero-nanostructures as catalysts for the CO_2RR for high-value C_{2+} products. The prepared Au@Cu_2O catalysts exhibit high catalytic performance due to the synergistic effects of Au and Cu. Furthermore, multiple interfaces between Au and Cu on the catalyst are produced by controlling the morphology to increase the enhanced active surface area and catalytic activity.

Poster Presentation : **MAT.P-669**

Material Chemistry

Event Hall THU 11:00~13:00

Structurally Ordered Pt-based Intermetallic Catalyst for Electrochemical Oxygen Reduction in Proton Exchange Membrane Fuel Cells

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[1]*Department of Chemistry, Korea University, Korea*

Designing the structurally ordered intermetallic nanostructure is an efficient strategy to significantly improve the catalytic performance of Pt-based electrocatalysts for oxygen reduction reaction (ORR) in fuel cells. In this study, we synthesized the ordered Pt-M intermetallic nanocatalyst by introducing the metal oxide shell on the Pt-based template materials. This metal oxide (MO_x) shell can provide abundant oxygen vacancies during the reduction process from MO_x to metallic species, which accelerate the interdiffusion of metal atoms, and prevent sintering of nanoparticles during thermal annealing at the high temperature. Furthermore, the maximizing charge redistribution between Pt and metal induces the high electron density and down-shifting of the d-band center on the Pt sites, resulting in the enhanced ORR activity. This study highlights the rational synthetic strategy for ordered Pt-based ternary intermetallic nanocatalyst by employing a bifunctional metal oxide shell instead of silica on the nanoparticles.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **MAT.P-670**
Material Chemistry
Event Hall THU 11:00~13:00

Single atom-modified Ru_2P nanocrystals for efficient hydrogen evolution reaction in alkaline media

Sangyeon Jeong, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Designing efficient electrocatalysts for hydrogen evolution reaction (HER) is crucial for renewable and sustainable energy conversion. Of particular importance is HER in alkaline media, which is vital to trade-off H_{ad}, hydroxyl adsorption$(OH)_{ad}$, and water dissociation. Therefore, the rational design of electrocatalysts with an excellent ability to dissociate water and bind hydrogen species can offer a pathway towards highly efficient alkaline HER catalysts. Significant progress has recently been made on constructing single atom modified catalysts, exhibiting much higher catalytic activity than non-modified catalysts towards HER due to the maximized utilization of atoms and the synergistic effects with the support materials. However, hybridizing single atoms into suitable host materials and isolating atoms into chemically distinct substances remains a significant challenge. Herein, we suggest that these limits can be resolved with a facile dual cation exchange strategy. we construct a series of Ru_2P nanocatalysts with atomically incorporated metals and investigated the correlation between the metal and catalytic performances. The superior catalytic performance of the M-Ru_2P catalysts via the atomic scale synergistic effect of metals and Ru_2P phase highlights the importance of atomic-level engineering strategy for electronic structure tuning of phosphide materials and boosting their catalytic properties effectively

Poster Presentation : **MAT.P-671**

Material Chemistry

Event Hall THU 11:00~13:00

Preparation of CuO-decorated carbon nanotubes and their photocatalytic characterization

Ji Dang Kim, Hyun Chul Choi*

Department of Chemistry, Chonnam National University, Korea

The cupric oxide (CuO) with a narrow band gap of 1.2 eV is one of the most widely studied photocatalysts due to its low cost, nontoxicity, abundant resource, and chemical stability. However, the conventional powder CuO has the high rate of photo-induced electron-hole recombination, which limited the formation of radicals on the surface of photocatalyst, resulting in low photocatalytic efficiency. Therefore, many methods have been explored to suppress the recombination rate of CuO. In this work, we prepared CuO-decorated carbon nanotubes (CuO-CNTs) by deposition of CuO on thiolated carbon nanotube (CNT) surfaces. Also, we investigated the effect of CNTs on the microstructure, physicochemical properties, and photocatalytic activity of CuO for the degradation of rhodamine B solution by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and transmission electron microscopy (TEM).

Poster Presentation : **MAT.P-672**

Material Chemistry

Event Hall THU 11:00~13:00

Chemical Vapor Deposition Growth of Amorphous Boron Nitride

HyeongJoon Kim, **Hyeon Suk Shin***

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea

Amorphous materials have been widely studied in many fields. Among them, amorphous boron nitride (aBN) has attracted attention because of its excellent electrical (ultra-low dielectric constant ~1.78, high breakdown field ~8.3 MV/cm) and mechanical property (high hardness ~ 11 GPa). In particular, its low dielectric constant value of less than 2 showed the potential for use as an interlayer dielectric (ILD in integrated circuits). However, a limitation of aBN study is that it is difficult to grow pure aBN thin films. In this presentation, we introduce the growth of aBN thin film by plasma enhanced chemical vapor deposition (PECVD). The grown aBN thin films were characterized by Raman, X-ray photoelectron spectroscopy (XPS), ellipsometry, and transmission electron microscopy (TEM). The characterization data indicated that aBN thin films include hBN nano-crystallites. We show the growth of aBN thin films with different amounts of hBN nano-crystallites and demonstrate how the crystallites affect the property of aBN.

Poster Presentation : **MAT.P-673**

Material Chemistry

Event Hall THU 11:00~13:00

Bright and Efficient Pure Red Perovskite Nanocrystal Light-Emitting Devices via In-situ Modification

Xinyu Shen, Zhongkai Yu, Woo Hyeon Jeong[1], Xiangyang Fan, Bo Ram Lee[*]

Department of Physics, Pukyong National University, Korea
[1]*Department of Chemistry, Hanyang University, Korea*

Although light-emitting devices (LEDs) based on metal halide perovskite nanocrystals (PNCs) developed rapidly in recent years, the luminance of pure red LEDs with the Rec.2020 standard Commission Internationale de l'Eclairage (CIE) 1931 color coordinates of (0.708, 0.292) cannot meet the requirement of outdoor display. Herein, a facile in-situ modification strategy was proposed to prepare the efficiently luminescent CsPb(Br/I)3 PNCs, where metal bromides were used to create a halide rich environment and inhibit the formation of nonradiative surface defects. Synchronously, appropriately increased surface ligands improved the effective exciton confinement. Hence, the modified CsPb(Br/I)3 PNCs exhibited a high PLQY of 92.0%. Additionally, the electrical conductivity was improved due to the increased hole mobility and the Auger process was inhibited caused by balanced carrier mobilities. Consequently, LEDs based on the modified CsPb(Br/I)3 PNCs exhibited a maximum luminance of 11233 cd m-2 with the pure red color coordinate (0.704, 0.292) and a peak EQE value of 13.2%. Furthermore, the luminance reached 5198 cd m-2 under the driving voltage of 4.4V. This is the first work to realize a pure red PNC LED with high luminance under low bias, which can meet the requirement of outdoor display.

Poster Presentation : **MAT.P-674**

Material Chemistry

Event Hall THU 11:00~13:00

Polymer/Small-Molecule Binary-Blend Hole Transport Layer for Enhancing Charge Balance in Blue Perovskite Light Emitting Diodes

Zhongkai Yu, Woo Hyeon Jeong[1], Xinyu Shen, Bo Ram Lee[*]

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Metal halide based perovskite light-emitting diodes (PeLEDs) are promising candidates for next generation commercial display products due to their excellent high color-purity and recent dramatic improvements in their device efficiencies. However, the performance of blue PeLEDs falls far short of the requirements of commercialization, for which one of the main reasons is a wide band gap of blue-emitting perovskites, resulting in inferior hole injection and imbalanced charge transport in the emissive layer. Here, we introduce a facile method for overcoming the charge balance issue by developing polymer/small-molecule binary-blend hole transport layer (HTL) with poly(9-vinlycarbazole) (PVK) and 2-(4-biphenyl)-5-(4-tert-butylphenyl)-1,3,4oxadiazole) (PBD). A simple but effective concept of the blended HTL allows a systematic modulation of hole injection barrier that enabled a balanced charge transport between electrons and holes for an effective recombination within perovskite emissive layer. In particular, the PeLED based on optimal blended HTL exhibits a high external quantum efficiency (EQE) of 5.30% with emission peak at 478 nm. Our work provides a simple and effective concept for forming an energy ladder for an efficient charge transport which will contribute towards developing high performance blue PeLEDs.

Poster Presentation : **MAT.P-675**

Material Chemistry

Event Hall THU 11:00~13:00

Physicochemical Understanding for the Impact of Pore Environment on Adsorption Behaviour: Finding and Understanding Reverse Sequential Pore Condensation of CO2 in MOF-205

Hae Sung Cho

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For better designing adsorbents, it is important to know the intermolecular interaction between adsorbate and host material, leading to guest selectivity and uptake capacity. In this study, we demonstrate the influence of the adsorbate-substrate interaction controlled by pore environment on the adsorption behaviour. Especially, we report the unique CO2 adsorption behaviour of MOF-205 due to distinct pore geometry. The precise analysis through gas adsorption crystallography with molecular simulation shows that capillary condensation of CO2 in MOF-205 occurs preferentially in large dodecahedral pore rather than small tetrahedral pore due to relatively weaker intermolecular interactions of CO2 with MOF-205 framework than those among CO2 molecules, while Ar and N2 are sequentially filled into two different pores of MOF-205 following their size as other MOFs. Comparison of adsorption of various porous materials with different pore geometry and chemistry reveals that the relative strength of adsorbate-adsorbate and adsorbate-substrate interaction controlled by pore environment gives rise to different shapes of adsorption isotherm, which can lead to a detailed physicochemical understanding of the influence of pore environments on the adsorption behaviour.

Poster Presentation : **MAT.P-676**

Material Chemistry

Event Hall THU 11:00~13:00

Thiol based Self-assembled monolayers on Zinc anodes for dendrite-free and stable plating and stripping in aqueous zinc-ion batteries

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Repeated charge/discharge in aqueous zinc-ion batteries (ZIBs) commonly results in surface corrosion/passivation and dendrite formation on zinc anodes, which are major challenges for the commercialization of zinc-based batteries. In this work, a self-assembled monolayer on zinc metal is described as a viable anode for ZIBs. A mercaptoundecanoinc acid which is spontaneously adsorbed on Zn surface is seen to suppress both dendrites and other side reactions in ZIBs. This is aided by the densely packed alkyl chains which prohibit direct contact of H2O and H^+ with underlying Zn, and surface carboxylate moieties ($-COO^-$) effectively repel anionic species (OH^-) in a solution, which renders a Zn anode inert against zincate formation. At the same time, the electrostatic attraction between surface-carboxylates and cations increases the concentration of Zn^{2+} on the modified Zn surface to facilitate Zn plating/stripping with less overpotentials. As a result, zinc modified by a monolayer shows excellent stability during prolonged Zn plating/stripping.

Poster Presentation : **MAT.P-677**

Material Chemistry

Event Hall THU 11:00~13:00

Comprehensive multi-variable Bayesian optimization for a new composition in Na_3PS_4 Family with superb Na^+ conductivity

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Na_3PS_4 is an archetype in room-temperature (RT) Na^+-conducting solid-state electrolytes. Various compositional modifications of this compound via iso/aliovalent substitution are known to have the high ionic conductivity (σ_{ion}) comparable to liquid electrolytes. In this work, we implement the Bayesian optimization (BO) algorithm to discover a new composition with high σ_{ion} in a multi-dimensional search space. The systematically designed search space used for our BO implementation consists of compositional variables ($A = Ca^{2+}, Y^{3+}, La^{3+}$; $M_1 = P^{5+}, Sb^{5+}$; $M_2 = Si^{4+}, Ge^{4+}, Sn^{4+}$; $Q = S^{2-}, Se^{2-}, Te^{2-}$; $X = Cl^-, Br^-, I^-$ in $(Na, A)_{3\pm\delta}(M_1, M_2, W)(Q, X)_4$) and processing variables (synthetic temperature and time). $Na_{2.81}(W_{0.22}Si_{0.10}Sb_{0.68})S_{3.93}Br_{0.07}$ selected through BO is further refined via logical reasoning, and finally Br^-free $Na_{2.88}(W_{0.22}Si_{0.10}Sb_{0.68})S_4$ is newly discovered. This heavily co-doped Na_3SbS_4 by Si^{4+} and W^{6+} shows high σ_{ion} of 20.2 and 7.4 $mS\cdot cm^{-1}$ at RT and -20°C, respectively, which is ascribed to the notably low activation barrier (0.14 eV) in Na_3SbS_4 families. Low electronic conductivity (2 x 10-10 $S\cdot cm^{-1}$) and stable Na plating/stripping behaviors are also disclosed, implying that $Na_{2.88}(W_{0.22}Si_{0.10}Sb_{0.68})S_4$ could be a promising SSE in Na_3SbS_4 families.

Poster Presentation : **MAT.P-678**

Material Chemistry

Event Hall THU 11:00~13:00

Enhanced performance by methylene-blue-doped TiO_2 under visible region

Gyeong-Ah Kim, **Kyung-Hun Park**[1,*]

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At present, a photocatalyst that can adsorb particulate matter (PM) with an electric charge is a popular method for PM reduction. Some commonly used photocatalysts comprise single metal oxides such as TiO_2 and ZnO, which could be utilized under ultraviolet (UV) region. However, because UV region constitutes a very small part of the total wavelength of sunlight, technology needs to be developed that allows the utilization of the visible region as well. Herein, we developed a new organic material that activated under not only UV region but also visible region by utilizing methylene blue (MB) with TiO_2. To make the TiO_2–MB film adsorb well, we discuss various solvents, concentration controls, and even coating methods. By conducting NO removal test, we showed that it is possible to reduce the PM more effectively by using TiO_2–MB film than that achieved using TiO_2 alone.

Poster Presentation : **MAT.P-679**

Material Chemistry

Event Hall THU 11:00~13:00

Stability and Efficiency Enhancement of Perovskite Solar Cells using Phenyltriethylammonium Iodide

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Controlling the perovskite film surface is key to improving both the stability and photovoltaic performance of perovskite solar cells. In particular, surface defects on the perovskite films, which are fundamental issues, must be passivated. In this work, we present a two-dimensional (2D) organic material phenyltriethylammonium iodide (PTEAI) to passivate a three-dimensional (3D) (FAPbI3)1-x(MAPbBr3)x perovskite film surface. PTEAI forms a well-matched conformal layer on the perovskite film, protecting the film surface from moisture by preventing the escape of organic ions from the film. The N+ cations and I- anions in PTEAI form bonds with the locally charged perovskite surface, reducing the surface defect density as well as the impeding non-radiative recombination while enhancing carrier lifetimes. We demonstrate that these PTEAI features facilitate significant enhancements in both the open-circuit voltage (Voc) and fill factor (FF) of the perovskite solar cells. As a result, the champion PTEAI-based perovskite solar cell exhibits the highest power conversion efficiency of 20.2% compared with 18.8% by the pristine device. Additionally, the PTEAI-treated device retains 92% of its initial efficiency after being stored in ambient air at room temperature and a relative humidity of 40–60% for 500 hours without encapsulation.

Poster Presentation : **MAT.P-680**

Material Chemistry

Event Hall THU 11:00~13:00

Highly efficient small molecule electron transport layer for solution processing in organic optoelectronic devices

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Optoelectronic devices with organic semiconductors, such as organic light- emitting diodes (OLEDs), have received rapid progress via solution-processing after years of effort. However, excellent device performance and cost-effective fabrication process are still necessary for practical applications. We designed a novel quinoxaline-phosphine oxide small molecules (QPSMs) utilized as the electron transport layer (ETL) for the solution-processable OLEDs . QPSMs can be dissolved in isopropanol owing to the strong dipole moments within their molecular structures, thereby resulting in an effective and convenient deposition on the emission layer without annealing. Furthermore, the electron injection/extraction was been improved in the QPSMs based device due to the well-matched energy levels in OLEDs. Especially, the optimized OLEDs with DMPQxTPPO1 exhibit external quantum efficiency (EQE) of 6.12% These results demonstrate that the QPSMs present a potential application value in organic semiconductor.

Poster Presentation : **MAT.P-681**

Material Chemistry

Event Hall THU 11:00~13:00

Cadmium Surface Passivation of Perovskite Nanocrystals for Blue LEDs

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Next-generation electroluminescent displays require efficient and stable light-emitting diodes (LEDs) with low cost, excellent color purity for which perovskites-based LEDs (PeLEDs) are a promising candidate. Among the three primary colors, the low efficiencies and poor stability of blue color PeLEDs is the major hurdle to their commercialization. Here, we demonstrate an surface engineering strategy incorporating a simple hot injection method with one pot synthesis for surface passivation of cadmium ions (Cd^{2+}) into blue-color all inorganic Cs base perovskite nanocrystals (PNCs). The optimized PNCs containing 0.2% Cd show improved photoluminescence quantum yield (PLQY; 66.8 %) and ambient stability, compared to the neat PNCs (25.5%) at an emission wavelength of 475 nm. PeLEDs with the PNC show a luminance of 51 cd/m^2 and EQE of 3.71%.

Poster Presentation : **MAT.P-682**

Material Chemistry

Event Hall THU 11:00~13:00

Monolayer Graphitic Carbon Nitride as Metal-Free Catalyst with Enhanced Performance in Photo and Electro-Catalysis

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The exfoliation of bulk graphitic carbon nitride (g-C_3N_4) into monolayer has been intensively studied to induce maximum surface area for fundamental studies, but ended in failure to realize chemically and physically well-defined monolayer of g-C_3N_4 mostly due to the difficulty in reducing the layer thickness down to an atomic level. It has, therefore, remained as a challenging issue in two-dimensional (2D) chemistry and physics communities. In this study, an “atomic monolayer of g-C_3N_4 with perfect two-dimensional limit” was successfully prepared by the chemically well-defined two-step routes. The atomically resolved monolayer of g-C_3N_4 was also confirmed by spectroscopic and microscopic analyses. In addition, the experimental Cs-HRTEM image was collected, for the first time, which was in excellent agreement with the theoretically simulated; the evidence of monolayer of g-C_3N_4 in the perfect 2D limit becomes now clear from the HRTEM image of orderly hexagonal symmetry with a cavity formed by encirclement of three adjacent heptazine units. Compared to bulk g-C_3N_4, the presentg-C_3N_4 monolayer showed significantly higher photocatalytic generation of H_2O_2 and H_2, and electrocatalytic oxygen reduction reaction. In addition, its photocatalytic efficiency for H_2O_2 production was found to be the best for any known g-C_3N_4 nanomaterials, underscoring the remarkable advantage of monolayer formation in optimizing the catalyst performance of g-C_3N_4.

Poster Presentation : **MAT.P-683**

Material Chemistry

Event Hall THU 11:00~13:00

Platinum-based Nanozyme: a Metastasis suppressor of Glioblastoma

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Nanozyme with enzymatic activities acts as direct surrogates of natural enzymes for catalysis. Compared with protein enzymes, it provides better catalytic stability and cost-efficient operation for production. Especially, biological activities of nanonzyme have been recognized as a cutting-edge tool in the field of anti-bacterial and anti-cancer, because the nanozymes could regulate intracellular factors such as pH, glutathione, and hydrogen peroxide (H2O2) in biological conditions. Glioblastoma (GBM), one of brain cancer, has a higher rate of mortality due to a high rate of recurrence after surgery. The recurrence is induced by high metastasis activities of GBM when the cavity occurs after resection of GBM. In this work, we report the anti-metastasis properties of a nanozyme that consists of hyperbranched polyamidoamine dendrimers (Sixth-generation) with encapsulation of platinum nanoparticles (called by Pt-dendrimer). We performed the synthesis and analysis of characterization for Pt-dendrimer. The Pt-dendrimer has a tiny size (< 10 nm), well-defined size (PDI < 0.3), potentials for surface functionalization, well-enzymatic function (H2O2 decomposition activities). With these excellent properties, we evaluated biological enzymatic functions in the normal and GBM cells. As a result, Pt-dendrimer showed outstanding performances in GBM cells even at a low concentration (0.5 μM); i) Anti-cancer, ii) Enzymatic function (H2O2 decomposition), iii) Anti-recurrence in 2D/3D analysis. To understand these activities of Pt-dendrimer, we confirmed the decrement at a level of mRNA related to metastasis of cancer. Given the biologically promising performances of Pt-dendrimer, we believed that Pt-dendrimer could be proposed as a new agent for inhibition of the recurrence of GBM.

Poster Presentation : **MAT.P-684**

Material Chemistry

Event Hall THU 11:00~13:00

Atom economy design of sub-2 nm Co3O4 ultra-small nanoparticles embedded porous carbon for enhanced and stabilized oxygen evolution from seawater.

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Most importantly, chemical free and noble metal free design of electrocatalysts is highly required. First time we have applied chemical free strategy to design highly reactive sub-2 nm Co3O4 ultra-small nanoparticles (USNPs) and active edges having 2dimensional fibrous carbon wrapped Co3O4 ultra-small nanoparticles (Co3O4 USNPs@FC). The strategy is the single green waste source (fibrous orange peel) for two utilities and multi applications (1+2+m) with zero waste generation. The green solvent with functional groups plays a crucial role to obtained Co3O4 ultra-small nanoparticles, which were further intertwined with the plethora of active sites have fibers carbon. Due to pivotal traits like high surface area, mesoporosity, and lone pair of electrons in the structure of Co3O4 USNPs@FC shows an excellent electrocatalyst activity for oxygen evaluation reaction (OER) with an overpotential of 390 mV at 10 mA cm-2 and high stability under seawater. This synthesis strategy unveils to create eco-friendly nanostructures for energy conversion from various aqueous systems.

Poster Presentation : **MAT.P-685**

Material Chemistry

Event Hall THU 11:00~13:00

Improved Organic Photovoltaic Performance with Quinoxaline-Based D-A Type Polymers by Systematic Modulation of Electron-Withdrawing Substituents

Jung Won Yoon, Hyosung Choi*

Department of Chemistry, Hanyang University, Korea

The advantages of polymer solar cell (PSC) such as semitransparency, flexibility, lightweight, and low-cost production. In a typical PSC, huge attention has been also paid to the development of p-type polymeric donors with appropriate energy levels, good carrier mobility, and favorable morphology for realizing high-performance PSCs. The polymer usually comprises alternating electron-donating (D) and electron-accepting (A) units along the polymer chain. Among various promising building blocks for D-A type polymers, in particular, quinoxaline moiety has emerged as a promising A component, because of its unique merits such as simple synthetic routes and facile structural variations. Additionally, its mild electron-accepting power fits well to prepare medium bandgap polymers. The combination of medium bandgap polymeric donors and narrow bandgap NFAs allows BHJ photoactive layers to exhibit beneficial complementary light absorption profiles. Herein, four D-A type polymers with multiple electron-withdrawing groups are designed and synthesized to be used for non-fullerene PSCs. In all polymers, the thienyl-substituted benzodithiophene (BDT) and quinoxaline with two fluorine atoms at meta-position of phenyl ring on 2,3-position were selected as a basic D and A building block, respectively. Afterward, the presence of fluorine atoms on the thiophene side chains of BDT donor, and the electron-withdrawing units of a fluorine atom or cyano group at the 5-position of quinoxaline acceptor were methodically controlled to investigate their effects on the photovoltaic properties of the polymers.

Poster Presentation : **MAT.P-686**

Material Chemistry

Event Hall THU 11:00~13:00

Solution-Phase Ligand Exchange of Perovskite Quantum Dot for Stable and Efficient Optoelectronics

Hochan Song, Hyosung Choi*

Department of Chemistry, Hanyang University, Korea

Semiconducting lead halide perovskite quantum dots (PQDs) are now experiencing a renaissance, stemming from their outstanding optoelectronic properties suited for optoelectronic applications. Invaluable endeavors have rapidly pushed up the performances of state-of-the-art PQD optoelectronics, especially for light-emitting diodes and photovoltaics. However, despite the solid-phase based surface management strategies demonstrating excellent PQD optoelectronics, these still involve deleterious effects to PQD surface and matrix, making further development more challenging. Here we devise a solution-phase ligand exchange protocol of the PQDs to effectively address all of the urgent issues by using aromatic ligands, where the aromatic ring of ligand plays a decisive role in surface passivation, dispersity, and phase stability of the PQD. The Solar cell device employing the PQD exhibit outstanding performances with unprecedent stability; a photovoltaic efficiency of 14.9 per cent with a single-step spin-coated PQDs that is intact upon ambient storage over 4 months. Density functional theory revealed that surface covering aromatic rings completely prevent the lattice from ambient moisture, responsible for the excellent phase stability. This work exemplifies how the aromatic rings control over surface chemistry of PQD in solution-phase without sacrificing solar cell performances and provides a straightforward route to dramatically overcome the notoriously labile stability of the materials and devices.

Poster Presentation : **MAT.P-687**
Material Chemistry
Event Hall THU 11:00~13:00

Hydrotalcite–Niclosamide Nanohybrid as an Anti-SARS-CoV-2 Strategy

Seungjin Yu, Huiyan Piao[1], Sanoj Rejinold Nirichan[1], Yehyun Kim[2], Goeun Choi[3,*], Jin-Ho Choy[4,*]

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COVID-19 has been affecting millions of individuals worldwide and, thus far, there is no accurate therapeutic strategy. This critical situation necessitates novel formulations for already existing, FDA approved, but poorly absorbable drug candidates, such as niclosamide (NIC), which is of great relevance. In this context, we have rationally designed NIC-loaded hydrotalcite composite nanohybrids, which were further coated with Tween 60 or hydroxypropyl methyl cellulose (HPMC), and characterized them in vitro. The optimized nanohybrids showed particle sizes

Poster Presentation : **MAT.P-688**

Material Chemistry

Event Hall THU 11:00~13:00

Niclosamide encapsulated in mesoporous silica and geopolymer: A potential oral formulation towards SARS-CoV-2 Viral Infections

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COVID-19 is a rapidly evolving emergency, for which there have been no specific medication found yet. Therefore, it is necessary to find a solution for this ongoing pandemic with the aid of advanced pharmaceutics. What is proposed as a solution is the repurposing of FDA approved drug such as niclosamide (NIC) having multiple pathways to inactivate the SARS-CoV-2, the specific virion that induces COVID-19. However, NIC is hardly soluble in an aqueous solution, thereby poor bioavailability, resulting in low drug efficacy. To overcome such a disadvantage, we propose here an oral formulation based on Tween 60 coated drug delivery system comprised of three different mesoporous silica biomaterials like MCM-41, SBA-15, and geopolymer encapsulated with NIC molecules. According to the release studies under a gastro/intestinal solution, the cumulative NIC release out of NIC-silica nanohybrids was found to be greatly enhanced to ~97% compared to the solubility of intact NIC (~40%) under the same condition. We also confirmed the therapeutically relevant bioavailability for NIC by performing pharmacokinetic (PK) study in rats with NIC-silica oral formulations. In addition, we discussed in detail how the PK parameters could be altered not only by the engineered porous structure and property, but also by interfacial interactions between ion-NIC dipole, NIC–NIC dipoles and/or pore wall-NIC van der Waals in the intra-pores of silica nanoparticles.

Poster Presentation : **MAT.P-689**

Material Chemistry

Event Hall THU 11:00~13:00

Organic-Inorganic Hybrid Perovskites: Synthesis, Stability and Optoelectronic Properties

Atanu Jana

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Organic-Inorganic Hybrid Perovskites: Synthesis, Stability and Optoelectronic Properties

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Lead halide perovskites (LHPs) with general formula ABX_3 (A = monovalent organic/inorganic cation, B = divalent metal cation, X = halide ion) are emerging as a promising material for several optoelectronic devices such as solar cells and light-emitting diodes. Especially, perovskite-based solar cells have the full potential to replace the Si-based solar cells as perovskites are solution-processable and exhibit high conversion efficiency from sunlight to electricity. But these materials degrade instantly in the presence of water due to their weak ionic bonding between organic and inorganic moieties. All-inorganic and organic-inorganic LHPs were first discovered in 1893 and 1978, respectively, and it remains a critical challenge for synthetic chemists to solve the instability issue. We solved this longstanding problem in 2018 without using any foreign surface passivating ligands. How? It will be discussed in my talk. Different kinds of synthetic routes are necessary to achieve the full potential of these materials. Traditionally, LHPs nanocrystals are synthesized by solution process using high boiling organic solvents that are expensive and environmentally hazardous. We have demonstrated a solvent-free mechanochemical synthetic route of LHPs nanomaterials and this procedure is gaining interest among the perovskite community. Mechanochemical synthesis is an attractive procedure with remarkable simplicity, rapidity, and reproducibility. We have also developed a synthetic route that can produce gram-scale quantity of LHPs nanomaterials. The bandgap of hybrid perovskites has also been tuned with a different synthetic approach by varying the A-site organic cations in ABX_3 LHPs. Details of these different synthetic routes and their potential benefits will be discussed along with the device applications such as solar cells and light-emitting diodes.

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Poster Presentation : **MAT.P-690**

Material Chemistry

Event Hall THU 11:00~13:00

High current density water-splitting catalyst for alkaline-anion-exchange-membrane water-electrolyzer

Abhishek Meena

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Among several alternative renewable energy technologies, splitting water to generate hydrogen for fuel is by far the most decent and viable technology that has gathered enormous interest in the recent few decades. Industrial water electrolyzers are a vital apparatus to produce pure hydrogen from water splitting. Alkaline anion and proton exchange membrane water-electrolyzers (AAEMWE and PEMWE) are primarily known as low- temperature water electrolyzer technologies. As yet, water electrolysis contributes only less than 5% to global hydrogen production due to practical and economic issues with the electrolyzer fabrication technologies. Therefore, the critical challenge is to develop highly efficient nonnoble metal catalysts for large-scale water splitting with low cell voltages towards commercialization. We report the design and synthesis of novel cost-effective Ni 2 P@FePOxHy nanoparticles (NPs) composite as a highly efficient OER electrocatalyst. Along with efficient HER catalyst in a highly corrosive environment (30% KOH) used for commercial water splitting, our catalyst achieves high j = 500 and 1000 mA cm -2 at 1.65 and 1.715 V, respectively, with long-term durability. Further, the catalyst delivers j = 1 A cm −2 at a cell voltage of 1.84 V in a commercial AAEMWE cell working with 1 M KOH, outperforming the commercially used Pt/C–IrO 2 catalyst. Details of high current density catalysts and their different synthetic routes and its potential benefits will be discussed along with the commercial applications in AAEMWE cells.References: 1. Chemical Engineering Journal 430, 132623 2. Applied Catalysis B: Environmental, 121127 3. Energy & Environmental Science 13 (10), 3447-3458

Poster Presentation : **ELEC.P-641**

Electrochemistry

Event Hall FRI 11:00~13:00

Wash- and Separation-Free Electrochemical Detection of *Porphyromonas gingivalis* in Saliva

Seonhwa Park, Haesik Yang*

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Indirect detection of *Porphyromonas gingivalis* in saliva, based on proteolytic cleavage by gingipain (Arg-gingipain), has traditionally been used for initial diagnosis of periodontitis. However, the traditional detection method using a colorimetry divides the concentration of *P. gingivalis* into positive, weakly positive, and negative only. Here, we report electrochemical biosensor for quantitative detection of *P. gingivalis* in saliva. An electrochemical active species, 4-aminophenol (AP), is liberated by the proteolytic reaction between a peptide substrate (glycine-proline-arginine conjugated with AP) and a gingipain which is a trypsin-like protease in the outer membrane of *P. gingivalis*. The electrochemical signal of AP was amplified by electrochemical-chemical redox cycling involving a indium-tin oxide electrode partially modified with multi-well carbon nanotubes, AP, and tris(2-carboxyethyl)phosphine. The electrochemical charge signal was corrected using the initial charge obtained before an incubation period. The calculated detection limit for *P. gingivalis* in artificial saliva was 5×10^5 CFU/mL, and the concentration of *P. gingivalis* in human saliva could be measured. The developed biosensor can be used as an initial diagnosis method to distinguish between healthy people and patients with periodontitis.

Poster Presentation : **ELEC.P-642**

Electrochemistry

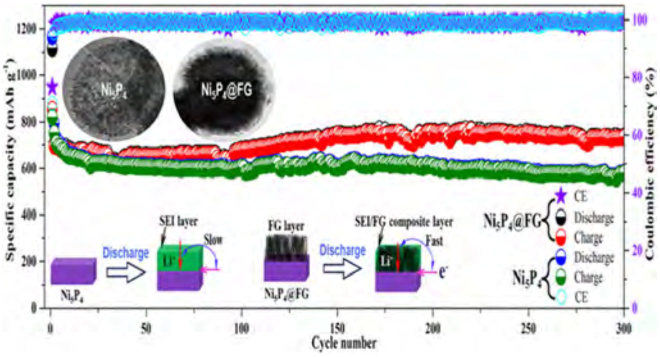
Event Hall FRI 11:00~13:00

Self-Templated Formation of Fluffy Graphene-Wrapped Ni5P4 Hollow Spheres for Li-Ion Battery Anodes with High Cycling Stability

Gisang Park, Jong-Sung Yu*

Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

Transition-metal phosphides have gained great importance in the field of energy conversion and storage such as electrochemical water splitting, fuel cells, and Li-ion batteries. In this study, a rationally designed novel fluffy graphene (FG)-wrapped monophasic Ni5P4 (Ni5P4@FG) is in-situ-synthesized using a chemical vapor deposition method as a Li-ion battery anode material. The porous and hollow structure of Ni5P4 core is greatly helpful for lithium-ion diffusion, and at the same time, the cilia-like graphene nanosheet shell provides an electron-conducting layer and stabilizes the solid electrolyte interface formed on the Ni5P4 surface. The Ni5P4@FG sample shows a high reversible capacity of 739 mAh g–1 after 300 cycles at a specific current density of 500 mA g–1. The high capacity, superior cycling stability, and improved rate capability of Ni5P4@FG are ascribed to its unique hierarchical structure. Moreover, the present efficient fabrication methodology of Ni5P4@FG has potential to be developed as a general method for the synthesis of other transition-metal phosphides.



Poster Presentation : **ELEC.P-643**

Electrochemistry

Event Hall FRI 11:00~13:00

[Withdrawal] Nitrogen-Doped Graphene Quantum Dots for the High Performance Lithium Sulfur Battery

Joonhee Moon

Research Center for Materials Analysis, Korea Basic Science Institute, Korea

- Withdrawal -

Poster Presentation : **ELEC.P-644**

Electrochemistry

Event Hall FRI 11:00~13:00

Trypsin Detection Employing Electrochemical Reduction-Based Redox Cycling

Hyo eun Lee, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

It is more difficult to achieve high signal-to-background ratios in biosensors using electrochemical reduction than using electrochemical oxidation. In this presentation, we propose a method for trypsin detection using electrochemical reduction-based redox cycling. Electrochemical-enzymatic (EN) redox cycling and electrochemical-chemical (EC) redox cycling for trypsin detection were tested and compared. Trypsin activates the EN and EC redox-cycling reactions by cleaving the peptide bond of electrochemically inactive p-aminophenol (AP)-conjugated oligopeptide, generating the electrochemically active AP. Horseradish peroxidase and cytochrome c (Cyt c) were tested as redox enzymes for EN redox cycling involving a redox enzyme and H2O2. With lower background levels, Cyt c showed better results than horseradish peroxidase. The trypsin detection based on the EN redox cycling involving Cyt c and H2O2 (~50 ng/mL) exhibited lower detection limits than the detection through EC redox cycling with IO3− (~100 ng/mL), due to its higher signal levels.

Poster Presentation : **ELEC.P-645**

Electrochemistry

Event Hall FRI 11:00~13:00

Sensitive and Low-background Electrochemical Immunosensor Using 1,10-Phenanthroline-5,6-dione and Glucose Dehydrogenase

<u>Young Jin Jung</u>, Haesik Yang[1,*]

Department of chemistry, Pusan National University, Korea

[1]*Department of Chemistry, Pusan National University, Korea*

We report a electrochemical immunosensor with high sensitive and low electrochemical background level, which results from electrochemical-enzymatic (EN) redox cycling based on mediated electrochemical oxidation of an electro-inactive reductant (glucose) at 0.0 V. The EN redox cycling employs flavin adenine dinucleotide-dependent glucose dehydrogenase and 1,10-phenanthroline-5,6-dione (PD). When PD was compared with five common quinone-based electron mediators, PD enabled the highest signal-to-background ratio, due to a very low electrochemical background level. When EN redox cycling was applied to a sandwich-type immunosensor, parathyroid hormone (PTH) in serum could be detected with a very low detection limit of ~0.1 pg/mL.

Poster Presentation : **ELEC.P-646**

Electrochemistry

Event Hall FRI 11:00~13:00

Formation of Nanoporous Gold on Ultramicroelectrode using Applying constant potential

Seoin Shin, Jongwon Kim[1,*]

Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Nanoporous gold (NPG) has a wide surface area due to nanometer-sized pores throughout the body and is being applied in various technical fields due to various other characteristics. In the experiment, NPG is formed by applying a constant potential for a certain period using UME as a working electrode. Rod electrode determines the potential to be applied through a scan and applies a constant potential for a certain period to form NPG. Unlike rod electrodes, UME forms NPG by applying 1.3V, which has the largest surface area, for a certain period because it cannot determine the voltage to be applied through scan. When NPG is formed in UME, the following experiment was conducted to find out whether the presence or absence of scan process the surface area of NPG. The experiment was conducted using 25 um UME, and the surface area was compared by forming NPG using the method of applying a constant potential after scanning and the method of applying only a constant potential. As a result, the surface area of the electrode became larger when applying a constant potential after scanning than when applying only a constant potential. Through this, it can be seen that scanning and applying a constant voltage when forming NPG in UME is efficient in forming a larger surface area.

Poster Presentation : **ELEC.P-647**

Electrochemistry

Event Hall FRI 11:00~13:00

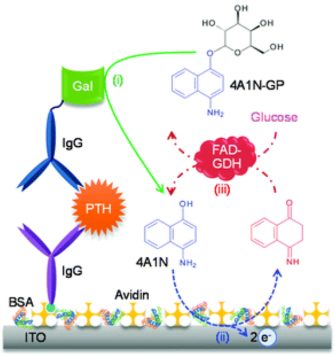
Sensitive electrochemical immunosensor using a bienzymatic system consisting of β-galactosidaseand glucose dehydrogenase

Jihyeon Kim, Haesik Yang[1,*]

Department of chemistry, Pusan National University, Korea

[1]*Department of Chemistry, Pusan National University, Korea*

Bienzymatic systems are often used with electrochemical affinity biosensors to achieve high signal levels and/or low background levels. It is important to select two enzymes whose reactions do not exhibit mutual interference but have similar optimal conditions. Here, we report a sensitive electrochemical immunosensor based on a bienzymatic system consisting of β-galactosidase (Gal, a hydrolase enzyme) and flavin adenine dinucleotide-dependent glucose dehydrogenase (FAD-GDH, a redox enzyme). Both enzymes showed high activities at neutral pH, the reactions catalyzed by them did not exhibit mutual interference, and the electrochemical-enzymatic redox cycling based on FAD-GDH coupled with enzymatic amplification by Gal enabled high signal amplification. Among the three amino-hydroxy-naphthalenes and 4-aminophenol (potential Gal products), 4-amino-1-naphthol showed the highest signal amplification. Glucose, as an electro-inactive, stable reducing agent for redox cycling, helped in achieving low background levels. Our bienzymatic system could detect parathyroid hormone at a detection limit of ~0.2 pg mL−1, implying that it can be used for highly sensitive electrochemical detection of parathyroid hormone and other biomarkers in human serum.



Poster Presentation : **ELEC.P-648**

Electrochemistry

Event Hall FRI 11:00~13:00

Permeabilization Using Tris buffer containing hydrazine for Sensitive Electrochemical detection of Aspergilus niger

Nakyeong Yoon, Haesik Yang[1,*]

Department of chemistry, Pusan National University, Korea
[1]*Department of Chemistry, Pusan National University, Korea*

It is challenging to turn redox metabolites present inside fungi into measurable signals using permeabilization because of the fungi's thick and rigid cell walls. We introduce that Aspergilus niger(A.niger) can be detected using the electrochemical measurement of redox metabolites excreted by a low level of permeabilization of the cell wall of A.niger, when incubated in tris buffer containing hydrazine. Electrochemical signals of redox metabolites are amplified by electrochemical-chemical redox cycling, in which hydrazine takes an initiating role as a reductant for rapid redox cycling. The detection process is specific to A.niger among the major three fungi triggering aspergilosis. The evaluated detection limit for A.nier is ~2 × 102 CFU/ml in spite of the incubation time being only 5 min, suggesting that the detection method is highly sensitive and rapid. The detection method does not need a wash step, specific affinity binding, or pretreatment step, indicating that it is a simple technique.

Poster Presentation : **ELEC.P-649**

Electrochemistry

Event Hall FRI 11:00~13:00

Simple and rapid Ag deposition method using a redox enzyme label and quinone substrate for the sensitive electrochemical detection of thyroid-stimulating hormone

Aman Bhatia, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Enzyme-induced seedless Ag deposition is useful for selective Ag deposition and subsequent electrochemical Ag oxidation; however, a washing step is required after the deposition and before the electrochemical oxidation as the enzyme substrate can be oxidized during the electrochemical oxidation. We report a fast Ag deposition method using a redox enzyme and quinone substrate that does not require a washing step. We found that the quinone substrate is reduced by a redox enzyme label, which is later oxidized to its original form via the reduction of Ag+ to Ag. Moreover, the quinone substrate is not electrochemically oxidized during the electrochemical Ag oxidation. We selected one diaphorase and 1,4-naphthoquinone from among seven redox enzymes (four diaphorases and three glucose-oxidizing enzymes) and six quinones, respectively. We applied this Ag deposition method for the detection of thyroid-stimulating hormone (TSH) over a dynamic range from 100 fg/mL to 100 ng/mL and found that TSH could be detected at concentrations as low as approximately 100 fg/mL in artificial serum. Therefore, the Ag deposition strategy developed in this study exhibits promising potential for ultrasensitive clinical applications.

Poster Presentation : **ELEC.P-650**

Electrochemistry

Event Hall FRI 11:00~13:00

Electro-inductive effect: Electrodes that act as functional groups to tune electronic properties of a molecule

Hojin Ahn, Sang Woo Han*

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

In place of functional groups that impose different inductive effects, we immobilize molecules carrying thiol groups on a gold electrode. By applying different voltages, the properties of the immobilized molecules can be tuned. The base-catalyzed saponification of benzoic esters is fully inhibited by applying a mildly negative voltage of –0.25 volt versus open circuit potential. Furthermore, the rate of a Suzuki-Miyaura cross-coupling reaction can be changed by applying a voltage when the arylhalide substrate is immobilized on a gold electrode. Finally, a two-step carboxylic acid amidation is shown to benefit from a switch in applied voltage between addition of a carbodiimide coupling reagent and introduction of the amine.

Poster Presentation : **ELEC.P-651**

Electrochemistry

Event Hall FRI 11:00~13:00

Wash-Free, Sandwich-Type Thrombin Detection Using Direct Electron Transfer and Catalytic Signal Amplification of Multiple Redox Labels

Gyeongho Kim, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Direct electron transfer (DET) between a redox label and an electrode has been used for sensitive and selective sandwich-type detection without a wash step. However, applying DET is still highly challenging in protein detection, and a single redox label per probe is insufficient to obtain a high electrochemical signal. In this presentation, we report a wash-free, sandwich-type detection of thrombin using DET and catalytic signal amplification of multiple redox labels. The detection scheme is based on (i) the redox label-catalyzed oxidation of a reductant, (ii) the conjugation of multiple redox labels per probe using a poly-linker, (iii) the low nonspecific adsorption of the conjugated poly-linker due to uncharged, reduced redox labels, and (iv) a facile DET using long, flexible poly-linker and spacer DNA. Amine-reactive phenazine ethosulfate and NADH were used as the redox label and reductant, respectively. N3-terminated polylysine was used as the poly-linker for the conjugation between an aptamer probe and multiple redox labels. Approximately 11 redox labels per probe and rapid catalytic NADH oxidation enable high signal amplification. Thrombin in urine could be detected without a wash step with a detection limit of ~50 pM, which is practically promising for point-of-care testing of proteins.

Poster Presentation : **ELEC.P-652**

Electrochemistry

Event Hall FRI 11:00~13:00

Fe-doped Cu_xRh_{1-x} Alloy Nanofibers as an Outstanding pH-universal Electrocatalyst for Hydrogen Evolution Reaction

Yoonhee Nam, Dasol Jin, Chongmok Lee[1], Youngmi Lee[*]

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

[1]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*

Under the various environmental issues and economic concerns caused by the use of fossil fuels, the development of sustainable and renewable energy has been required. In particular, sustainable hydrogen production from water splitting, central to the area of renewable energy conversion, is attracting attention as a carbon-neutral energy conversion system. Considering the growing attention to water electrolysis, the developing electrocatalysts with cost-effectiveness and long-term stability for hydrogen evolution reaction (HER) has been studied in recent years. In current work, Fe-doped single spinel $CuRh_2O_4$ nanofibers are synthesized by electrospinning and post-calcination process with various doping content of Fe. Through the subsequent thermal hydrogen reduction, Fe-doped Cu_xRh_{1-x} nanofibers are prepared. Physical characteristics of the elemental compositions and surface morphologies are analyzed through field-emission scanning electron spectroscopy (FE-SEM), energy dispersive X-ray spectrometer (EDS), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). The crystalline structures of the prepared nanomaterials are investigated through high-resolution X-ray diffraction (XRD). Electrochemical measurements for the synthesized Fe-doped Cu_xRh_{1-x} nanofibers are carried out with rotating disk electrode (RDE) voltammetry focused on HER performance under a wide pH range of aqueous solutions (*i.e.*, KOH, PBS and H_2SO_4). This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : **ELEC.P-653**

Electrochemistry

Event Hall FRI 11:00~13:00

Improvement in Ionic Conductivity of a Composite Polymer Electrolyte via 1,1-Diethyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles for All-solid-state Batteries

Hyeong Rok Si, Se Yeon Park, Ji Hun Lee, Young Tae Park[1,*]

chemistry department, Keimyung University, Korea

[1]*Department of Chemistry, Keimyung University, Korea*

To reduce the safety drawbacks of liquid electrolyte-based Li-ion batteries, there is a growing intrigue in the evolution of solid-state electrolytes (SSEs) based Li-metal batteries. Unfortunately, most SSEs have low ionic conductivity (σ), which notably lowers the performance of the Li-metal batteries. However, the composite polymer electrolyte (CPE) endows a higher σ value, which still needs to be supplemented for a reliable Li-metal battery. Here, 1,1-diethyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles (Et_TMSA) was used as a filler. The polyethylene oxide (PEO) and LiTFSI were used as substrate and Li-salt, respectively. The cross-link between the silole crystal and the PEO crystal makes the movement of lithium more smooth. Thus, the value of σ was greatly improved, which help to make better interfacial contact with the electrodes. The CPE electrolyte with 2 wt% Et_TMSA provided an outstanding σ value of 1.09×10^{-3} S/cm (@60 ℃). Apart from, the achieved discharged specific capacities were 154 mAh/g using LiFePO4 cathodes at the discharge current density of 0.1 C. These results indicate that composite polymer electrolytes containing silole material could be a potential alternative for solid-state Li-metal batteries. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

Poster Presentation : **ELEC.P-654**

Electrochemistry

Event Hall FRI 11:00~13:00

Ruthenium-Chromium Mixed Oxide Core-Shell Nanofibers for Highly Efficient Oxygen Evolution Reaction Catalysis under pH-Universal Condition

Chaewon Song, Yoonkyeong Kim, Dasol Jin, Chongmok Lee, Youngmi Lee*

Department of Chemistry & Nano Science, Ewha Womans University, Korea

Hydrogen fuels have been considered as one of the most promising substitutes for fossil fuels due to their environment-friendly products. Electrochemical water splitting is an efficient way for hydrogen production. However, the efficiency of water electrolysis for hydrogen production is mainly degraded by the complex reaction mechanism and slow kinetics of oxygen evolution reaction (OER), which is a half-reaction coupled to hydrogen evolution reaction (HER). Electrocatalysts with outstanding activity for OER mostly depend on noble metal (e.g. Ir, Ru, and Pt) catalysts. However, the industrial applications of these noble metals are impeded due to their rareness and high cost. Therefore, the significance of high-performance electrocatalysts is emphasized to reduce the kinetic barrier of OER and improve energy efficiency.Herein, we synthesize ruthenium (Ru)-chromium (Cr) mixed oxide core-shell nanofibers via electrospinning and calcination process. Synthetic conditions such as calcination atmosphere are controlled to alter the actual structures of Ru-Cr core-shell nanofibers. Physical properties are analyzed by FE-SEM, EDS, XRD, and TEM. Electrocatalytic performances of Ru-Cr mixed oxide core-shell nanofibers are evaluated with rotating disk electrode (RDE) voltammetry under acidic, neutral, and alkaline conditions to figure out their activities toward OER under pH-universal conditions. The OER activities of synthesized Ru-Cr oxide core-shell nanofibers are characterized in a relation with the structures. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : **ELEC.P-655**

Electrochemistry

Event Hall FRI 11:00~13:00

Fabrication of porous Pt films by Electrochemical deposition using polystyrene beads

Changhee Lee, Jongwon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

Platinum is known to have good electrochemical catalyst activity, but it has the disadvantage of being rare and expensive. Therefore, in order to obtain high electrochemical catalytic activity with a small amount of platinum, research is conducted to make platinum with a nanoporous structure with a large electrochemical surface area (ESA). In this study, templates were formed using polystyrene beads of 2 μm and 1 μm in diameter, and platinum films having micro-level pores were made on the templates by electrochemical deposition. As a result, as the electrodeposition charge increased, the thickness of the platinum films increased, and accordingly, the ESA of platinum films calculated using H UPD also increased. In addition, as a result of measuring the oxygen evolution reaction (OER) activity using the platinum films, it was confirmed that the OER activity was increased compared to OER activity of bare Pt. However, as a result of measuring the ESA and OER activity of the platinum films stacked flat by electrochemical deposition without using the polystyrene bead, the ESA and OER activity were larger than that of the porous platinum films fabricated using the polystyrene beads. Therefore, further research will be needed in the future, but fabricating metal films having large ESA using the polystyrene bead templates by electrochemical deposition is expected to create various porous metal films by applying various sizes of polystyrene beads and various metals.

Poster Presentation : **ELEC.P-656**

Electrochemistry

Event Hall FRI 11:00~13:00

Molybdenum-Iridium Mixed Oxide Nanotubes as a pH-universal Electrocatalyst for Oxygen Evolution Reaction

Sunghwa Ahn, Dasol Jin, Chongmok Lee, Youngmi Lee*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

To meet the carbon-neutral energy needs of modern society, a lot of research to develop renewable and environment-friendly energy generation was carried out. One of the ways to generate hydrogen fuel is water splitting including oxygen evolution reaction (OER). OER involves four electrons/protons coupled for the reaction and requires high overpotential to overcome the kinetic energy barrier. Accordingly, the interest in exploiting efficient and low-cost catalysts for OER has been increased. Here, we present the synthetic process and physical/electrochemical characterization of molybdenum-iridium mixed oxide ($Mo_xIr_{1-x}O_3$) nanotubes as electrocatalysts for OER in a wide range of pH. $Mo_xIr_{1-x}O_3$ nanotubes are synthesized via electrospinning followed by calcination process. Interestingly, the rate of thermal calcination process can control the diameter of the $Mo_xIr_{1-x}O_3$ nanotubes. The morphology and composition of the synthesized materials are characterized by FE-SEM, EDS, HRTEM and XPS. Their crystalline structures are investigated through XRD. Electrochemical measurements of $Mo_xIr_{1-x}O_3$ nanotubes are performed with rotating disk electrode (RDE) voltammetry in Ar-saturated pH-universal (*i.e.*, KOH, PBS and H_2SO_4) aqueous solution with different molar concentration (*i.e.*, 1.0, 0.5 and 0.1 M) to evaluate OER performances. This research was financially supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : **ELEC.P-657**

Electrochemistry

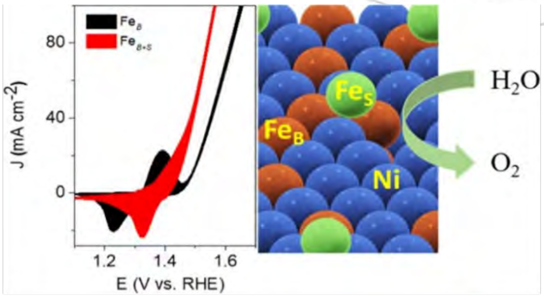
Event Hall FRI 11:00~13:00

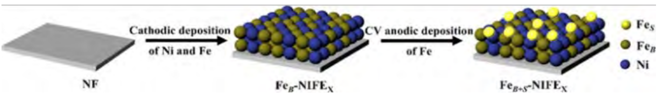
Synthesis and application of ultrathin Ni–Fe LDH nanosheets for efficient electrochemical water splitting

Goddati Mahendra

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, Korea

Abstract: In an electrochemical water splitting, developing a cost-effective, abundant and highly efficient electrocatalyst is a major challenge for the large-scale production of hydrogen and oxygen gasses. Recently, applications of transition-metal based layered double hydroxides as electrocatalyst in water splitting have attracted attention because of their abundance, stability and environmental friendliness. Here, an ultrathin nickel-iron layered double hydroxide (NiFe-LDH) nanosheet was synthesized through electrodeposition onto nickel foam (NF) substrates. In alkaline solution, the as-synthesized ultrathin nanosheet has exhibited an excellent oxygen evolution activity. Combined with its lower overpotential of 240 mV at 10 mAcm-2 and turnover frequency at an overpotential of 400mV, and durability over 15, 000 s, this material is a promising electrocatalyst for water splitting.Keywords: amorphous, bulk and surface Fe, integrated, NiFe oxyhydroxide nanosheets, oxygen evolution reaction





Poster Presentation : **ELEC.P-658**

Electrochemistry

Event Hall FRI 11:00~13:00

Toward high-voltage and low self-discharge by utilizing deep eutectic solvent as an electrolyte of Redox-enhanced Electrochemical Capacitors.

Dahye Kim, JinHyuck Ko, JInhwan Byeon[1], Seung Joon Yoo*

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea
[1]*School of Chemistry, Gwangju Institute of Science and Technology, Korea*

In recent years, a system with higher power than a battery and higher energy than a capacitor is being actively studied. One of the promising approaches is to develop aqueous redox-enhanced electrochemical capacitors (Redox ECs). Redox ECs improve energy using the redox reactions of redox-active molecules dissolved in the liquid-state electrolyte. An aqueous electrolyte is safe, environmentally friendly, and has high conductivity. But this system is restricted by the small electrochemical stability window of water and a fast self-discharge due to cross-diffusion.In this presentation, we solved the chronical problems of the aqueous-based electrochemical capacitors by using a deep eutectic solvent (DES). DES is a promising green electrolyte due to being non-flammable, low-cost, biodegradable, and non-toxic. Herein, Ethaline (choline chloride and ethylene glycol mixed) was used as a DES electrolyte to utilize a wide ESW of over 2 V. Further, by adding ethyl viologen dibromide (EVBr) as a redox-active molecule, the specific energy of this redox EC reached 48.96 Wh/kg at 0.5 A/g with over 90% coulombic efficiency. This system can suppress fast self-discharge by trapping the reduced ethyl viologen through the pores of the ethaline due to the change in the solvated shell size of the reduced ethyl viologen. our system utilizing redox DES shows 25.99% energy retention at 18 hr open-circuit time, while aqueous-based system maintains just 8.39% of energy retention.

Poster Presentation : **ELEC.P-659**

Electrochemistry

Event Hall FRI 11:00~13:00

Highly soluble Quinone redox-enhanced electrochemical capacitors utilizing hydrotropic supporting electrolyte assisted solubility enhancement

JinHyuck Ko, Seung Joon Yoo*, JInhwan Byeon[1]

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea
[1]*Gwangju Institute of Science and Technology, Korea*

Redox-enhanced electrochemical capacitors (redox ECs) provide increased energy density by utilizing the faradaic reactions of redox molecules dissolved in the electrolyte. The solubility of redox molecules is directly related to the cell performance in a redox EC. Unfortunately, most commonly used redox molecules have a low solubility in an aqueous system. In order to solve this solubility issue, a complex and costly synthetic process involving substitution of derivatives has been required and practiced. In the present work, we introduce the novel concept of hydrotropic supporting electrolyte (HSE) that can act as both a hydrotrope and a supporting electrolyte simultaneously. By adding the HSE, we report a 7-fold increase in the solubility of hydroquinone (HQ) compared with that of HQ in the conventional 1M H_2SO_4 aqueous electrolyte. Based on the HQ solubility enhancement results, we newly synthesized triethanol ammonium substituted anthraquinone (AQM) for further enhancing the performance of redox ECs. We also discover that there are two different solubility enhancing mechanisms (pre-Ouzo structure, quasi-micelle structure) of the hydrotrope depending on the interaction between the hydrotrope and functional group of the redox molecules. Based on the new understanding of using hydrotrope as a HSE, we successfully developed a dual-redox EC consisting of a bromide catholyte and an AQM anolyte with the addition of p-TsOH as an HSE. This system provides a specific energy of ~40 Wh/kg at 2 A/g and maintains 90% energy retention over > 2000 cycles. Our research will give a guideline for improving the solubility of the all quinone series redox molecules for the development of a high-energy and high-stability redox-EC system.

Poster Presentation : **ELEC.P-660**

Electrochemistry

Event Hall FRI 11:00~13:00

Energy Enhanced Hybrid Supercapacitors with cation and Concentration optimized Acetate-based WiSE(Water in Salt Electrolytes)

Subin Lee, Seung Joon Yoo*

School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Korea

Alkali metal ions have been widely investigated as a charge carrier in energy storage devices such as supercapacitors and batteries. Particularly, a lot of attention to utilizing K+, Na+ in aqueous electrolytes has been made due to their low cost, abundant reserves as well as smaller hydration radius compared to Li+ that results in higher ionic conductivity. In contrast, non-alkali metal ion such as ammonium ion (NH4+) is rarely considered although having similar ionic radius and hydrated radius to K+, and even higher ionic conductivity. In addition, ammonium ions can form hydrogen bonds, which proposes their chemical interactions in the electrolyte would be significantly distinct compared to that of alkali metal ions, potentially improving cell performance. In this presentation, we chose NH4OAc and KOAc as model electrolytes which are highly soluble in water, inexpensive, and both have environmentally benign acetate anions for fair cation comparison. First, we determine optimum concentration (herein referred as “pre-WiSE (Water in Salt Electrolyte)” to maximize ionic conductivity and stability of aqueous electrolyte. Assuming the gap of performance resulting from different chemical interaction (e.g. Hydrogen bonding) of K+ and NH4+, comparative study has been carried out by evaluating aqueous-based supercapacitor using pre-WiSE based on potassium acetate (KOAc) and ammonium acetate (NH4OAc). Furthermore, iodide was exploited as redox active additive to enhance insufficient energy density of aqueous double-layer based supercapacitors. This work offers not only the comparison of cations (K+ vs NH4+) in aspect of electrolyte chemistry, but also performance optimization of aqueous-based supercapacitors.

Poster Presentation : **ELEC.P-661**

Electrochemistry

Event Hall FRI 11:00~13:00

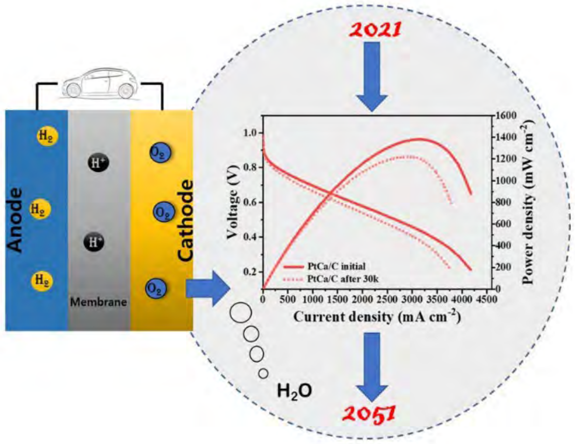
New and Novel PtCa/C catalyst as a Durable Cathode Material for Hydrogen Fuel Cell.

Gyan-Barimah Caleb, Jong-Sung Yu[1,*]

Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Ghana

[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Alloys of platinum-alkaline earth metals have been identified to be active and highly stable owing to their high negative alloy formation energies, but their synthesis in nanoparticulate form has proved challenging, which has discouraged most researchers from exploring this area. Our group reports for the first time the synthesis, characterization, and PEMFC test of PtCa nanoparticles prepared through the solution phase technique in an air-deficient environment. The PtCa catalyst reported here exhibits significant mass activity of 0.67 A/mgPt at 0.9 V in half-cell, with negligible activity decay in practical fuel cells over 30000 cycles according to the DOE protocol. This catalyst system holds great potential for the transportation industry.



Poster Presentation : **ELEC.P-662**

Electrochemistry

Event Hall FRI 11:00~13:00

Selectivity control of photoelectrochemical hypochlorous acid production on WO_3 photoelectrode

So Yeong Jo, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

Chloride ions are oxidized into reactive chlorine species such as Cl_2, HOCl, and OCl^-, which are strong oxidizing agents and are widely used for water disinfection. As an anodic half reaction of electrochemical water splitting, the oxidation of chloride ions is a promising alternative to the oxygen evolution reaction (OER) because it has a fast kinetic compared to the OER, and can also produce value-added products. In this work, the role of co-catalysts on WO_3 photoelectrode has been investigated to control product selectivity during photoelectrochemical reaction in a 0.5 M NaCl solution. Various catalysts were applied to the WO_3 microplates to investigate their catalytic activity and selectivity. The WO_3 microplates as a photoanode showed an improved HOCl production with decreased OER in the presence of Pt co-catalyst. On the other hand, the OER is maximized on the WO_3 microplates with Mn_3O_4 co-catalyst. The effects of co-catalysts, pH, and wavelength of light were fully investigated to understand the selective oxidation process. This study proposes the importance of catalysts and their applications to WO_3 electrode for selective and effective photoelectrochemical seawater splitting reactions.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ELEC.P-663**

Electrochemistry

Event Hall FRI 11:00~13:00

Hierarchical coral-like NiFe nanostructures as efficient oxygen evolution reaction

Sunguk Noh, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

The oxygen evolution reaction (OER) is a half-reaction process that determines the efficiency of electricity-driven water splitting due to its slow four-electron transfer kinetics and large overpotential. Much effort on developing OER catalysts with high activity and durability has been devoted for alkaline water electrolysis, which is one of the most promising solutions for future clean energy systems of hydrogen-fuel generating technologies. In this presentation, hierarchical coral-like NiFe nanochains with uniform spheres with an average diameter of ~450 nm was synthesized by a two-step procedure. As a template, highly uniform Ni nanochains composed of spherical nanoparticles with lengths of up to 3-7 μm was first synthesized via a simple reflux method. Subsequently, hierarchical coral-like NiFe layered double hydroxides (LDHs) were grown directly on Ni nanochains. The electrocatalytic activity of the obtained LDH nanochains for OER in alkaline media was investigated by rotating disk electrode, rotating ring disk electrode, and cyclic voltammetry. The hierarchical nanoarchitecture as well as porous structure benefit the material in electrochemical OER performance. The prepared catalysts were characterized with various analytical techniques to examine the structural features: field-emission scanning electron microscopy, high-resolution transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy.

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Poster Presentation : **ELEC.P-664**
Electrochemistry
Event Hall FRI 11:00~13:00

Electrochemical Nitrate Reduction to Ammonia on Polycrystalline Copper Electrodes in Alkaline solutions

Yohan Kim, Shim Minyoung, Hye Ryung Byon*

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Ammonia is widely used as a raw material for fertilizers and is supplied to fuel cells and hydrogen storage materials. In general, the Haber-Bosch process mass-produces ammonia($N_2 + H_2 \rightarrow 2NH_3$). However, this chemical process requires high-temperature and high-pressure conditions to decompose triple N_2 bond, and produces unwanted CO_2 gas because CH_4 is added for H_2 production. It is attractive to produce ammonia in ambient conditions and more cost-effective ways. In addition, the use of inevitably produced waste and ecotoxic species is also valuable as reactants. To this end, the conversion of nitrate (NO_3^-) using an electrochemical method is drawing attention. Nitrate is highly soluble in aqueous condition, and more reactive than N_2 gas at ambient temperature and atmospheric condition. Nevertheless, the nitrate reduction undergoes several electron transfer processes and causes low ammonia selectivity competing with by-products such as hydrogen gas, nitrogen oxides and hydroxylamine. Here, we show important factors in determining the conversion selectivity of nitrate using a Cu catalyst. We prepared three Cu films treated with other surface cleaning processes. The surface morphology and roughness of Cu dependent on surface treatment significantly changed the conversion efficiency. In particular, nitrogen oxide (NO) was sensitive to the Cu surface condition as it was a pivotal intermediate product that determines the final product. I will discuss details of the electrochemical nitrate reduction process observed by in-situ and ex-situ gas and spectroscopic analyses and correlate the conversion efficiency with the surface conditions of Cu foils.

Poster Presentation : **ELEC.P-665**

Electrochemistry

Event Hall FRI 11:00~13:00

Impact of Intrinsic Defects: Lithiation Behavior of n-Type and p-Type TiO_2

Geun Jun Lee, Jin Ho Bang[1,*], Muhammad Awais Abbas[2,*]

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[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*
[2]*Nanosensor Research Institute, Hanyang University, Pakistan*

TiO_2 has been used as anode material in lithium-ion batteries (LIBs) instead of graphite. However, it has some issues related to low lithium diffusion and electrical conductivity. To enhance these characteristics, control of intrinsic defects is one of the effective methods. It is possible to form two different defects in TiO_2, which are anionic and cationic. We compared oxygen vacancy (V_O) to titanium vacancy (V_{Ti}) of TiO_2. In this report, we controlled the synthesis process to exclude other crystal structure and morphology factors that are also possible to impact electrochemical performance. V_O in TiO_2 provides additional lithiation sites that increase capacity at low C-rates, but this over-lithiation makes a negative effect on cycling stability. Compared to V_O, V_{Ti} improves the rate performance and cycling stability of TiO_2 because of suppressing the over-lithiation. This defect control approach can be helpful to open a new path for high-performance TiO_2 as Lithium-ion batteries.

Poster Presentation : **ELEC.P-666**

Electrochemistry

Event Hall FRI 11:00~13:00

Electrochemical monitoring of liquid/liquid interfacial kinetics through single-entity electrochemistry

Hyeongkwon Moon, Jun Hui Park*

Department of Chemistry, Chungbuk Natioanl University, Korea

The new application of single nanodroplet electrochemistry to in situ monitor the interfacial transfer kinetics of electroactive species across liquid/liquid interface was reported. Interfacial kinetic information is crucial in drug delivery, the cosmetic industry, and membrane transport. However, interfacial information has been mainly studied thermodynamically, such as partition coefficient, which could not manifest a speed of transfer. Herein, we measure the phase-transfer kinetic constant via the steady-state electrochemistry of an extracted redox species in a single nanodroplet. The redox species were transferred from the continuous oil phase to the water nanodroplet by partition equilibrium. The transferred redox species are selectively electrolyzed within the droplet when the droplet contacts with an ultramicroelectrode, while the electrochemical reaction of the redox species outside the droplet (i.e., organic solvent) is effectively suppressed by adjusting the electrolyte composition. The redox species in the water droplets can quickly attain a steady-state during electrolysis owing to an extensive mass transfer by radial diffusion, and the steady-state current can be analyzed to obtain kinetic information with help from the finite-element method. Finally, a quick calculation method is suggested to estimate the kinetic constant of phase transfer without simulation.

Poster Presentation : **ELEC.P-667**

Electrochemistry

Event Hall FRI 11:00~13:00

Chemical and Electrochemical Phase Transformations of Cobalt Hydroxide for Electrochemical Water Splitting

Joon Yong Park, So Yeong Jo, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

Synthesizing individual cobalt hydroxides from an identical starting material may aid in discerning the relationship between the crystal structure and catalytic activity. Herein, the crystal structure of α-$Co(OH)_2$ and its transformation into other cobalt hydroxides were investigated. In particular, α-$Co(OH)_2$ comprised a layered structure with anion intercalation, which was identified by Rietveld refinement analysis. This corresponds to the chemical formula, $[CoOh_{0.77}\ CoTd_{0.23}\ (OH)_{1.77}]^{0.23+}[Cl_{0.23}\cdot 0.64H_2O]$. Chemical phase transformations of metastable α-$Co(OH)_2$ into various other cobalt hydroxides, such as β-$Co(OH)_2$, γ-CoOOH, and β-CoOOH, were selectively performed, and their structures were characterized. In addition, electrochemical oxidative phase transformations of α-$Co(OH)_2$ and β-$Co(OH)_2$ into γ-CoOOH and β-CoOOH, respectively, were successfully accomplished. Interestingly, electrochemical cation intercalation occurs only when the structure changes from α-$Co(OH)_2$ to γ-CoOOH. The cations in the electrolyte were selectively inserted into the layered structure to form the γ-CoOOH phase. The prepared cobalt hydroxides were subjected to the oxygen evolution reaction (OER) and chloride oxidation reaction (COR) to discern the correlation between the crystal structure and activity. The γ-CoOOH showed better OER catalytic activity than β-CoOOH. In contrast, β-CoOOH showed higher COR selectivity than γ-CoOOH at low chloride concentrations. The importance of the crystal structure for each electrocatalytic reaction is elucidated.

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Poster Presentation : **ELEC.P-668**

Electrochemistry

Event Hall FRI 11:00~13:00

RuCx Nanosurfaces as Hydrogen Evolution Reaction Electrocatalysts

Hee Jin Kim, Jeonghyeon Kim, Sang-Il Choi*

Department of Chemistry, Kyungpook National University, Korea

Although metastable crystal structures have received much attention owing to their utilization in various fields, their phase-transition to a thermodynamic structure has attracted comparably little interest. In the case of nanoscale Ru crystals, such an exothermic phase-transition releases high energy within a confined surface area and reconstructs surface atomic arrangement in a short time. Thus, this high-energy nanosurface may create novel crystal structures when some elements are supplied. In this work, the phase-transition process of cubic-close-packed to hexagonal-close-packed creates a new ruthenium carbide (RuC_x) phase on the surface of Ru nanocrystals. When the electrocatalytic hydrogen evolution reaction (HER) is tested in alkaline media, the RuCx phase on the surface of Ru nanocatalyst exhibits lower overpotential, smaller tafel slope, higher exchange current density and lower charge transfer resistance than the counterpart Ru-based catalysts and the state-of-the-art Pt/C catalyst. To obtain further insight into the new RuC_x phase, its electrocatalytic performance was tested in the presence of thiocyanate ions, confirmed that the RuC_x phase on the surface is active site. Density functional theory calculations predict that the local heterogeneity of the outermost RuC_x surface promotes the bifunctional HER mechanism by providing catalytic sites for both H adsorption and facile water dissociation.

Poster Presentation : **ELEC.P-669**

Electrochemistry

Event Hall FRI 11:00~13:00

Zn^{2+}-imidazole Coordination Crosslinks for Elastic Polymeric Binders in High Capacity Silicon Electrodes

Kiho Park, Jang Wook Choi[*]

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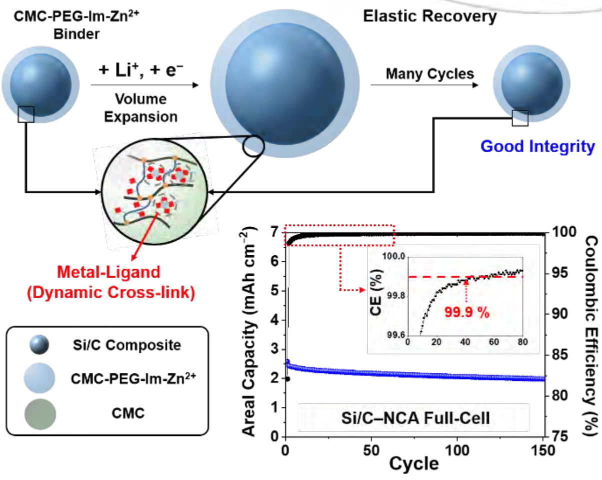
Recent research has built a consensus that the binder plays a key role in the performance of high-capacity silicon anodes in lithium-ion batteries. These anodes necessitate the use of a binder to maintain the electrode integrity during the immense volume change of silicon during cycling. Here, we report Zn^{2+}-imidazole coordination crosslinks that are formed to carboxymethyl cellulose (CMC) backbones in situ during electrode fabrication. The recoverable nature of Zn^{2+}-imidazole coordination bonds and the flexibility of the poly(ethylene glycol) chains are jointly responsible for the high elasticity of the binder network. The high elasticity tightens interparticle contacts and sustains the electrode integrity, both of which are beneficial for long-term cyclability. These electrodes, with their commercial levels of areal capacities, exhibit superior cycle life in full-cells paired with $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ cathodes. The current study underlines the importance of highly reversible metal ion-ligand coordination chemistries for binders intended for high capacity alloying-based electrodes.



Poster Presentation : **ELEC.P-670**

Electrochemistry

Event Hall FRI 11:00~13:00

Cross communication and pH perturbation in the vanadium oxide-based aqueous zinc ion batteries

Yangmoon Kim, Jang Wook Choi*

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Aqueous zinc ion batteries are receiving increasing attention for large-scale energy storage systems owing to their attractive features with respect to safety, cost, and scalability. Although vanadium oxides with various compositions have been demonstrated to store zinc ions reversibly, their limited cyclability especially at low current densities and their poor calendar life impede their widespread practical adoption. Herein, we reveal that the electrochemically inactive zinc pyrovanadate (ZVO) phase formed on the cathode surface is the main cause of the limited sustainability. Moreover, the formation of ZVO is closely related to the corrosion of the zinc metal counter electrode by perturbing the pH of the electrolyte. Thus, the dissolution of VO2(OH)2−, the source of the vanadium in the ZVO, is no longer prevented. The proposed amalgamated Zn anode improves the cyclability drastically by blocking the corrosion at the anode, verifying the importance of pH control and the interplay between both electrodes.

Poster Presentation : **ELEC.P-671**

Electrochemistry

Event Hall FRI 11:00~13:00

Highly Elastic Binder for Improved Cyclability of Nickel-Rich Layered Cathode Materials in Lithium-Ion Batteries

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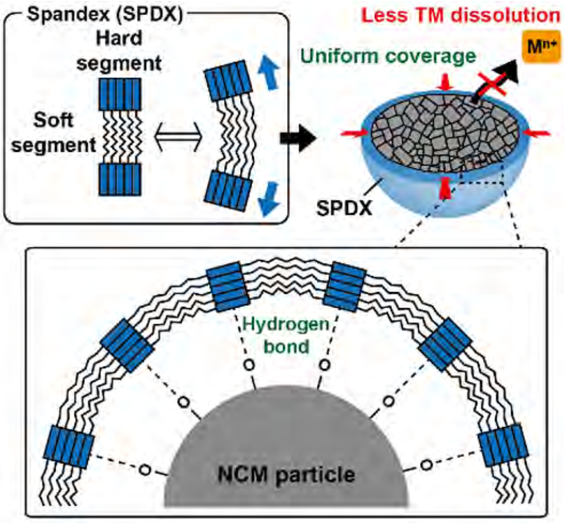
Among the cathode materials in lithium-ion batteries (LIBs), nickel (Ni)-rich layered cathode materials are currently receiving the most attention from the battery community due to their high specific capacities (~200 mAh g-1) and minimal use of high-cost cobalt. However, the high Ni content is disadvantageous in that it impairs cycling and structural stability. The chemically unstable Ni3+ can be deduced to Ni2+, which can migrate from the transition metal (TM) layer to the Li layer. This phenomenon is known as cation mixing and causes performance degradation in the cycle life, rate performance, and safety. Moreover, the long-term cyclability is adversely affected by amplified side reactions with carbonate-based electrolyte, which triggers unwanted interfacial reactions via catalytic and complexation routes and thus destabilizes the cathode-electrolyte interphase. Herein, it is reported that a highly elastic binder, namely spandex, can overcome the problems of Ni-rich layered cathode materials and improve their electrochemical properties drastically. The highly elasticity of spandex allows it to uniformly coat LiNi0.8Co0.1Mn0.1O2 (NCM811) particles via shear force during slurry mixing to protect the particles from undesired interfacial reactions during cycling. The uniform coating of spandex, together with its hydrogen bonding interaction with NCM811 leads to enhanced particle-to-particle interaction, which has multiple advantages, such as high loading capability, superior rate and cycling performance, and low binder content. This study highlights the promise of elastic binders to meet the ever-challenging criteria with respect to Ni-rich layered cathode materials in cells targeting electric vehicles.


Spandex (SPDX)
Hard segment
Soft segment
Less TM dissolution
Uniform coverage
M^{n+}
SPDX
Hydrogen bond
NCM particle

Poster Presentation : **ELEC.P-672**

Electrochemistry

Event Hall FRI 11:00~13:00

Design of Naphthalene Diimide for Highly Soluble and Stable Negolyte in Neutral Aqueous Organic Redox Flow Batteries

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Aqueous organic redox flow batteries (RFBs) have been extensively investigated as emerging energy storage systems. Because the current vanadium RFBs have suffered from the rising cost of elemental vanadium and precipitation of Vsup>5+ at > 40 oC, the development of alternative redox-active materials is urgently needed. The design of organic redox molecules can offer electrochemical stability, increasing solubility, and tunable redox potentials. We previously demonstrated that potassium salt of N, N'-bis(glycinyl)naphthalene diimide (NDI) showed stable two electrons transfer in aqueous RFBs (J. Mater. Chem. A 2020, 8, 11218). However, the solubility was very low at 25 mM under the neutral condition. Herein, we show the significantly improved solubility of NDI to ~1.5 M in water by incorporating four quaternary ammonium groups, indicated as ANDI. ANDI was stable during the two electron-transfer processes. As-prepared ANDI molecules were repelled due to the cationic ammonium groups in the neutral electrolyte solution. After the first reduction process, the electron paramagnetic resonance (EPR) signal was negligible despite the formation of ANDI radicals. It suggested the formation of radical π–dimer, where two NDI radical cores were close. The second reduction process produced monomeric dianion due to the repulsion of the anionic NDI cores. Moreover, the NDI core was attracted to the cationic ammonium wings, forming three-dimensional inter-molecular structures. The inter- and intra-molecular interactions of ANDIs during multiple electron transfers were attributed to excellent capacity retention in RFB tests. Aqueous RFBs consisted of 1 M ANDI as the negative electrolyte (negolyte), NH4I as the positive electrolyte (posolyte), and KCl as the supporting electrolyte. The full cell showed an average voltage of 1.08 V and stable cyclability 500 times, which took 45 days. A capacity-fading rate was estimated to be 0.004% per cycle, and a negligible crossover of ANDI was observed. This study demonstrated variable molecular structures and improved chemical stability of organic redox molecules in RFBs.

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Electrochemistry

Event Hall FRI 11:00~13:00

Fluorinated Carbonate derived Interface Formation for Stable Lithium Metal Batteries

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[1]Seoul National University, Korea

Lithium (Li) metal anode is among the most promising anodes with its high energy density. However, Li dendrites growth issues from heterogeneous solid electrolyte interphase (SEI) have been hindered the practical application of lithium metal batteries (LMBs) in portable electronics and electric vehicles. Herein, unsolvated fluorinated carbonate derived interface formation by solvation preference of ether co-solvent is proposed for stable lithium metal anodes. Ether solvent was introduced into fluorinated carbonate solvent, altering the solvation sheath of lithium ions, and the mixture of them showed the most enhanced interfacial stability and cycling performance. The remarkable achievement is attributed to the gradual decomposition of fluorinated carbonate on the electrodes, and the solvation chemistry of the electrolyte was further explored by density functional theory calculations. This work provides fresh insight into regulating the Li solvation sheath for stable SEI by solvation dominance difference between solvent molecules and demonstrates a guidance in rational electrolyte design for safe LMBs.

Poster Presentation : **ELEC.P-674**

Electrochemistry

Event Hall FRI 11:00~13:00

2D Material Based MXene-GO Protective Layer for Dendrite-Free Lithium Metal Anode

Sujin Kim, Jang Wook Choi*

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Lithium metal is a promising anode for next-generation battery systems to enable high energy density storage by replacing the currently used graphite anode. However, the practical application of Li anode has been hindered by the unstable solid electrolyte interphase and dendritic Li growth, which results in low Coulombic efficiency and poor cycling stability. Forming protective layers on Li anode is one of the effective strategies to stabilize the interface by introducing desired properties of diverse materials. Here, we demonstrate a 2D material-based protective layer composed of MXene and GO by a simple vacuum filtration method. The protective layer exhibits a uniform layered structure and remains stables during long-term stripping/plating of Li. The 2D materials, MXene and GO, can enhance the value of ionic conductivity and wettability of the interface through oxygen functional groups, resulting in decreased interfacial resistance after cycling. Additionally, the high mechanical strength and layered structure of 2D materials suppress the dendritic growth, promoting lateral Li deposition to achieve a dendrite-free Li metal anode. With this protective layer, long cycle life and high Coulombic efficiency are achieved for Li metal battery, and this work highlights the ability of 2D material-based protective layer in stabilizing Li metal anode.

Poster Presentation : **ELEC.P-675**

Electrochemistry

Event Hall FRI 11:00~13:00

Entropymetry for detecting micro-cracks of high-nickel layered oxide cathodes

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School of Chemical and Biological Engineering, Seoul National University, Korea

With an explosive increase of electric vehicles (EVs), non-destructive monitoring of degradation in lithium ion batteries became more important for real-time diagnosis of EVs. As demand for increase of mileage, high-nickel cathodes have been adopted while high-nickel cathodes suffer from various degradation such as micro-cracks. Here, we introduce entropymetry for monitoring the structural change of NMC811 cathode along the state of charge (SOC) and structural degradation. Entropy change corresponded with structural change during charge, especially at the 4.2V region which occurs a sharp reduction of c-axis lattice. Entropy change at the 4.2V region decreased after degradation, which was attributed to heterogeneity of sites for lithium ions due to structural degradation from cation mixing and micro-cracks. In-situ XRD estimated structural heterogeneity through peak broadness at the 4.2V region. Heterogeneity from structural degradation causes the reduction of equivalent energy states for Li ions and results in decrease of configurational entropy. Entropy change shows conditions of structural heterogeneity from different voltage cut-off and cycle number. The present study proposes entropymetry as the non-destructive tool for detecting micro-cracks of high-nickel layered oxide cathodes in lithium ion batteries.

Poster Presentation : **ELEC.P-676**

Electrochemistry

Event Hall FRI 11:00~13:00

Ruthenium anchored on carbon nanotube electrocatalysts for hydrogen production with enhanced Faradaic efficiency

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To electrochemically produce pure and clean hydrogen, the development of efficient and stable electrocatalysts is essential. A facile and economical synthetic method of electrocatalysts for the hydrogen evolution reaction (HER) is crucial for industrial applications. Herein, we demonstrated that ruthenium (Ru) nanoparticles uniformly anchored on multi-walled carbon nanotubes (MWCNTs) catalyst is capable of catalyzing HER. The catalyst showed the excellent catalytic activity with overpotential of 13 and 17 mA at a current density of 10 mA cm^{-2} in 0.5 M H_2SO_4 and 1.0M KOH, respectively, which is superior to commercial Pt/C of 16 and 33 mV. Furthermore, the catalyst has outstanding durability in both solutions, showing almost no loss during cycling test. In a real device, the hydrogen production of the catalyst per power consumption was 15.4% higher than Pt/C and Faradaic efficiency of the catalyst (92.28%) also was higher than Pt/C (85.97%). Density functional theory (DFT) calculations identified the catalyst comprising the Ru-C structure have appropriate hydrogen binding energies for HER, and strong Ru−C bonding energies reflects the excellent stability.

Poster Presentation : **ELEC.P-677**

Electrochemistry

Event Hall FRI 11:00~13:00

Influence of Applied Bias to Perovskite Quantum Dot Placed in Various Surroundings with Charge Transfer Process

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All-inorganic CsPbX3 (X: Cl, Br, or I) perovskite quantum dots (PQDs) are one of alternative materials to apply them in various optoelectronic devices and solar driven chemistry due to their outstanding photophysical properties such as high photoluminescence quantum yield (PLQY, >90%), high absorption cross section (> 105 cm-1), bandgap modulation, and so on. Our recent studies have elucidated that the PQDs are influenced by applied bias to transform the lead halide plumbate complexes. The reason was that the injected electrons and holes could induce the internal electron-phonon interactions (polarons) so that the polarons stimulated the irreversible transformation of the PQDs. In this study we further moved on the effect of electron transport medium (ETM) to the PQDs placed under the applied bias. By soaking the excited electrons to the ETM, we further investigated the in-situ/ex-situ photophysical/material properties of the PQDs under placed in the applied bias with contact to the ETM.

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Poster Presentation : **ELEC.P-678**

Electrochemistry

Event Hall FRI 11:00~13:00

Fabrication of a Triple Amperometric Sensor for Measurements of Nitric Oxide, Carbon Monoxide and Hydrogen Sulfide

Hyeji Yoon, Youngmi Lee*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Nitric oxide (NO), carbon monoxide (CO), and hydrogen sulfide (H_2S) known as some of the representative gasotransmitters are endogenously produced in living organisms and play vital roles in physiological and pathological conditions. These gases also commonly mediate vasorelaxation, neurotransmission, neuromodulation, inflammation, etc. Furthermore, NO, CO and H_2S closely interact with one another and control the other's biological generating process. In this research, we fabricate a triple amperometric microsensor for simultaneous measurements of NO/CO/H_2S. The sensor body consists of three working electrodes: 50-µm, 150-µm and 50-µm diameter Pt disks (WE1, 2 and 3, respectively). The WE1 is used to detect NO and its platinum surface is coated with NO selective membranes. Gold and iron are electrochemically co-deposited on WE2 for sensing CO and then its surface is loaded with CO selective membranes. The WE3 for H_2S sensing is electrochemically etched to make micropores and that space is stuffed with gold by electrodeposition. Then, a proper polymer is electropolymerized on WE3. These variations of each electrode's surface composition are important for enhancing sensitivity to its target gas and selectivity over interferences. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : **ELEC.P-679**

Electrochemistry

Event Hall FRI 11:00~13:00

The Photoinduced Electron Transfer Process in between Perovskite Quantum Dots Covered by Silica Medium and Transparent Conducting Oxide Monitoring through Spatially Resolved Time-correlated Single Photon Counting Method.

Jo Hyeonyeong, Sumi Seo, Seog Joon Yoon[*]

Department of Chemistry, Yeungnam University, Korea

All-inorganic cesium lead halide perovskite quantum dots (CsPbX3, X: Cl, Br, and/or I, called as PQDs) have been proved their potentials to utilize them into the optoelectronic devices and solar driven chemistry. However, to practically apply them into the applications, it is necessary to obtain stabilities against to photoirradiation, humidity, and so on. We have been tried to improve the stability of the PQDs by covering them through silica medium and obtained both stability and enhanced photocatalytic degradation of carcinogens. Going to one-step further, we tried to show the photoinduced electron transfer process in between the PQDs@SiOx and electron accepting materials (transparent conducting oxide, TCO) monitoring through spatially resolved time-correlated single photon counting tool. By differentiating the bandgap of the PQDs, we were able to obtain the evidences of photoinduced charge transfer from the PQDs@SiOx to TCO for all the cases of red-, green-, and blue- PQDs@SiOx.

Poster Presentation : **ELEC.P-680**

Electrochemistry

Event Hall FRI 11:00~13:00

Effect of Solvents to $CsPbBr_3@SiO_x$ Core-shell Perovskite Quantum Dots: Role of the Solvents for Material and Photophysical Properties of the $CsPbBr_3@SiO_x$ Quantum Dots

Sumi Seo, Jo Hyeonyeong[1], Seog Joon Yoon[2,*]

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[1]*Yeungnam University, Korea*
[2]*Department of Chemistry, Yeungnam University, Korea*

All-inorganic lead halide perovskite quantum dots (PQDs, $CsPbX_3$, X: Cl, Br, and/or I) have demonstrated their potential to various applications such as solar cells, light emitting diodes, solar driven chemistry, and so on. By controlling sizes up to exciton Bohr radius, the 0D PQDs open more various applications to sensors, biochemistry, lasing, *etc.*,. To make the PQDs, wet chemistry based synthetic strategies were applied and more device fabrications were utilized. In the wet chemistry, using solvents are inevitable but sometimes researchers do not interest about that how the solvents could affect to overall performance of the materials. In this work, we studied how various polar/non-polar solvents affect the material stability as well as photophysical properties of the $CsPbBr_3@SiO_x$ Core-shell PQDs.

Poster Presentation : **ELEC.P-681**

Electrochemistry

Event Hall FRI 11:00~13:00

Nitrogen-containing nanofilm on Cu electrode to achieve high activity of electrochemical CO_2 reduction

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[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Carbon dioxide (CO_2) emission from the combustion of fossil fuel causes global warming and climate change. Much attention has been paid for recycling of CO_2 gas, namely converting this greenhouse gas to high-value fuels such as multi-carbon products (ethylene, ethanol, propanol, etc.). In particular, electrochemical CO_2 reduction reaction (CO_2RR) is one of the promising methods operated at ambient pressure and room temperature. By using gold and silver catalysts, carbon monoxide (CO) is successfully yielded with >80% Faradaic efficiency. In contrast, it is still challenging to produce multi-carbon (i.e., C_{2+}) products. Copper (Cu) is known as the sole catalyst to yield C_{2+} products by affording the suitable binding energy to the intermediate of *CO (the asterisk denotes the surface adsorption). However, the selectivity of the desired product is low on the bare Cu foil-like electrode. It is attributed to hydrogen evolution reaction (HER) competing with CO_2RR. Additionally, the Cu surface is rapidly deactivated by dissolution, adsorption, and aggregation of Cu atoms, resulting in transformation of surface structure and morphology. To mitigate these problems, the interface modifications of Cu electrode are needed. As the well-known d-band center model has not been perfectly applied for CO_2RR, our strategy is to add Lewis-basicity-tunable organic film as the model adlayer to Cu electrode and investigate C_{2+} selectivity through tuning of CO_2 adsorption energy and intermediates of CO_2RR. Here, we show the enhanced CO_2 reduction activity and stability of Cu electrodes by introducing nitrogen-rich flat nanofilm (NF) on the Cu surface. The bare Cu electrode were prepared on Si wafer by electron-beam evaporation method, and the two different kinds of nanofilm, consist of similar structure with different nitrogen contents, indicated as N_0- and N_3-NF for the absence and the presence of nitrogen-containing heterocycle, was synthesized by photon-assisted imine condensation reaction between aldehyde and amine. After the reaction, formation of imine bond was proved by the FT-IR and X-ray photoelectron spectra. Thickness of the nanofilm was ~26 nm, confirmed by cross-sectional scanning electron microscopic (SEM) image. In addition, it was also confirmed by SEM image

that these nanofilms remained on the Cu surface even after vigorous electrolysis, supporting the good stability of the nanofilm. In the 2h of CO_2 reduction at -1.15 V vs. RHE, N_0-NF coated Cu showed 20% lower Faradaic efficiency (FE) towards H_2, compared to bare Cu. Furthermore, N_3-NF coated Cu showed half of FE for H_2, and 4-fold increased FE_{C2+}/FE_{C1} ratio. This result suggests that the nitrogen-containing heterocycle in the nanofilm can modify the electronic structure of the surface, and strengthen the adsorption energy of the CO_2 reduction intermediate. In this presentation, I will discuss the role of Lewis-basicity-tunable organic film in detail.

Poster Presentation : **ELEC.P-682**

Electrochemistry

Event Hall FRI 11:00~13:00

Investigation of Pd-doped Copper Hydride Nanocluster Electrocatalysts for Hydrogen Evolution Reaction

Eunsaem Park, Dongil Lee[1,*]

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Hydrogen fuel is clean source that have high energy density and considered as a promising candidate to replace fossil fuels. Electrochemical water splitting powered by renewables is a green way to produce hydrogen. Hydrogen evolution reaction (HER) is the fundamental process of water splitting, and it is necessary to develop highly active and low-cost catalyst for HER. In this study, we investigate HER activity of Pd-doped copper hydride nanoclusters, $[Cu_{11}PdH\{S_2P(O^iPr)_2\}_6(C\equiv CPh)_4]$ and $[Cu_{14}PdH_2\{S_2P(O^iPr)_2\}_6(C\equiv CPh)_6]$. (abbreviated as $Cu_{11}PdH$ and $Cu_{14}PdH_2$, respectively). The Pd-doped copper hydride nanoclusters were characterized by UV-Vis spectroscopy and mass spectrometry. The HER performance of $Cu_{11}PdH$ and $Cu_{14}PdH_2$ were compared by linear sweep voltammetry, electrochemical impedance spectroscopy, and Tafel slope analysis. The catalytic activity of $Cu_{11}PdH$ is much higher than $Cu_{14}PdH_2$, where the overpotentials for the 10 mA cm^{-2} of each nanocluster was 50 mV and 450 mV, respectively. Moreover, the hydrogen turnover frequency (TOF) determined for the $Cu_{11}PdH$ nanocluster was 250 s^{-1} at the overpotential of 100 mV, which is comparable to the best Pt-based single atom catalysts. This high catalytic activity implies that $Cu_{11}PdH$ have the advantage of the unique open surface structure and enabling the full utilization of the doped Pd atom.

Poster Presentation : **ELEC.P-683**
Electrochemistry
Event Hall FRI 11:00~13:00

Electrocatalytic Enhancement of Oxygen Reduction Activity Through MOF Confinement

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Metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) are extended structures consisting of metal ions or metal clusters and organic linkers. The steady increase in global energy demand and the depletion of fossil fuels has motivated researchers to focus on clean and sustainable energy conversion and storage materials. The fuel cell technology is the one going to balance the future energy demands due to its environmental sustainability and promising conversion efficiency. Due to the several required characteristics, this research field is still ceaseless, to address this here our target is to find a suitable catalyst material based on MOF confinement for oxygen reduction reaction (ORR). For the past three decades, pore-/cavity possessing crystalline materials, such as molecular containers, zeolites have been explored for various confined chemical transformations. In which the chemical reactions occur in a confined space with spatial restrictions as advantages to get the unprecedented products or increase the reaction rate. In the present study, we choose a highly porous and stable MOF, NU-1000, [$(Zr_6(\mu_3\text{–}OH)_8(OH)_8(TBAPy)_2)$, TBAPy = 1,3,6,8-tetrakis(p-benzoic acid)pyrene] as a host material and Ni-based square planar complex, Ni-ATP, [$Ni(atp)_2$, atp = 2-aminothiophenol] as an electrocatalyst (guest). The Ni-ATP complex was successfully incorporated inside the pores of NU-1000 MOF via the solution phase synthesis. The integrated material (Ni-ATP@NU-1000) was characterized by various analytical methods. The UV-Visible absorption spectrum and elemental mapping analysis of Ni-ATP@NU-1000 confirm the incorporation Ni-ATP quantitatively and qualitatively, respectively, and uniform distribution of the Ni-ATP complex in the MOF crystal. The decrease of the BET surface area and the pore volume also confirms the presence of Ni-ATP complex in the pores of the NU-1000 MOF. The quantity of Ni-ATP incorporation in the MOF was found to be ~ 200 mg/g. Furthermore, the quantity of Ni-ATP complex leaching from the Ni-ATP@NU-1000 solution is observed to be negligible under the wide range of pH. Based on these results the integrated material can be explored as a good electrocatalyst for ORR reactions. In addition, the effect of ORR activity with the various size ranges of MOF from nanometer to micrometer is under investigation. The interaction between the electron-rich pyrene linker of the MOF with the redox-active complex may lead to the formation of electro-catalytically active material thus enhancing the electrocatalytic activity. This study will provide a new path to understanding real electrocatalytic reaction mechanisms for ORR.

Poster Presentation : **ELEC.P-684**

Electrochemistry

Event Hall FRI 11:00~13:00

Tailoring Intrinsic Properties of Catalyst for Elevating CO_2 Reduction Performances into CO in Membrane Electrode Assembly

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Electrochemically CO_2 to CO conversion has achieved nearly 100% CO selectivity by certain metal-based catalysts before, and it is one step closer to industrialization by securing stability and performance. Also, the introduction of a GDE-based MEA and flow cell overcomes the low CO_2 solubility and achieves currents of several hundred mA cm^{-2}. Noble metal-based catalyst such as Ag, Au, and Zn have intensively been studied as an electrocatalyst for CO production from electrochemical CO_2 reduction reaction (eCO_2RR). Alloyed and nanostructure catalyst have been designed to control the intrinsic properties of catalysts. Also, halides could be another candidate for modifying the catalyst surface morphology.Here, we simply prepared AuAg alloy nanoparticle by galvanic replacement. The AuAg alloy catalyst made by incorporating Au species into Ag metal through the galvanic exchange has a high surface area, and the surface-active site controlled by Au significantly increased the activity of the catalyst. By Controlling diffusion rate of the Ag^+ ion through increased synthesis reaction temperature, AuAg alloy catalysts were synthesized in the form of AgCl on the catalyst surface and implemented between AuAg metal. We demonstrate that an intermetallic catalyst modified with Au on Ag achieves 90% CO selectivity and 437.2 mA cm^{-2} in a MEA cell. Furthermore, the catalyst covered by AgCl induces a morphological change in nanoparticles via reduction reaction, which greatly contributes to eCO_2RR selectivity and activity.

Poster Presentation : **ELEC.P-685**
Electrochemistry
Event Hall FRI 11:00~13:00

Detection of Attoliter Droplets Collision and Recollision via Single Entity Electrochemistry

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We monitored the dynamics of a single collided droplet with the ultramicroelectrode surface. Droplets were observed by amperometric i-t curve which was sequentially applying oxidative-reductive potentials. Potassium ferrocyanide, as redox indicator, was dissolved in aqueous phase would be oxidized when an aqueous droplet collided to UME which oxidative potential was applied. The reductive collision spikes were observed when the reductive potential is applied at UME immediately after oxidation. The reductive collision spikes were as the direct evidence because the redox species was dissolved in reduced form. Finally, the droplet properties were analyzed.

Poster Presentation : **ELEC.P-686**

Electrochemistry

Event Hall FRI 11:00~13:00

Development of High Energy Dual-Redox Electrochemical Capacitors utilizing Two-Electron Process of Viologen and Bromide.

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Aqueous redox-enhanced supercapacitors (redox SCs) are a type of supercapacitor that exhibits long-term cycling performance and high power density. Redox SCs additionally produce high energy density due to having dissolved redox active materials that participate redox reaction in the electrolyte. Also, aqueous electrolyte has a non-flammability, eco-friendliness and fast ion conductivity, thus redox SCs have received increasing research interest. However, there are still critical obstacles to overcome such as lower energy density with low operating voltage compared to secondary metal ion-based batteries and self-discharge issues due to cross-diffusion of dissolved redox species.In this work, we present dual redox system to maximize cell performance by using bromide and substituted viologens. With systematically structuring different substituents onto viologen redox core, we achieved the high energy density by using two-electron transfer reaction from the 6-hydroxyhexyl(6-OH) viologen. Compared to the one-electron transfer process, the amount of electron transferred is doubled with more negative redox potential of the negative electrode. This strategy is beneficial to the increase in energy density and further expand operating voltage up to 1.8V. In addition, studies on cross-diffusion and cycle stability according to the change of substituents of the viologen will be discussed.

129th General Meeting of the Korean Chemical Society
April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ELEC.P-687**

Electrochemistry

Event Hall FRI 11:00~13:00

Nitrogen-Doped Graphene Quantum Dots: Sulfiphilic Additives for Lithium Sulfur Batteries

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The lithium−sulfur cell is considered to be the most promising next-generation energy storage system. However, the practical use of Li−S batteries is hindered by several problems such as poor cycle retention, low Coulombic efficiency, low sulfur loading, and so forth. We herein for the first-time propose nitrogen-doped graphene quantum dots as the sulfiphilic additive for the advancement of Li−S cell performance. We carry out direct decoration of conducting additives and carbon cloth interlayers with graphene quantum dots and nitrogen-doped graphene quantum dots, which are evaluated in Li−S cells. Nitrogen doped graphene quantum dots exhibit strong sulfiphilic properties, and therefore, they anchor the liquid-phase polysulfides. The Li−S cell using the nitrogen-doped graphene quantum dot-decorated carbon cloth interlayer shows a discharge capacity of 1454.4 mA h gS−1 at 0.1 C and a capacity retention of 98.2% at 0.5 C after 300 cycles even with a sulfur loading of 6.0 mg S cm−2. Our study demonstrates that the nitrogen-doped graphene quantum dot is a promising additive, which can improve the viability of Li−S cells for the next generation of energy storage systems.

Poster Presentation : **ELEC.P-688**

Electrochemistry

Event Hall FRI 11:00~13:00

Maximizing the Strength of Electro-inductive Effect through Multi-linkage

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Electro-inductive effect (EIE), reported in 2020, is a concept that controls an electronic property of substrates using electrodes as functional groups. We can tune an electronic density on covalently bound substrates as functional groups do by applying a voltage to the electrode. Under given electrochemical reaction conditions, we have designed a multiple-linkage system for maximizing EIE with minimizing side reactions. For analysis, the correlations between the applied voltage and pKa value of immobilized molecules with single and dual linkages were obtained through the Henderson-Hasselbalch equation and surface-enhanced Raman spectroscopy. As a result, a difference in the correlation depending on the number of links shows that the substrate having dual linkages experience a more enhanced EIE than a single linkage. This finding also supports the evidence of the electro-inductive effect by demonstrating the acidity control of the immobilized molecule.

Reference

[1] Heo, J.; Ahn, H.; Won, J.; Son, J. G.; Shon, H. K.; Lee, T. G.; Han, S. W.; Baik, M.-H. Science 2020, 370, 214–219.

Poster Presentation : **ELEC.P-689**

Electrochemistry

Event Hall FRI 11:00~13:00

Hierarchical Carbon Nanosheets Decorated with Ruthenium Nanoparticles for Deformable Electrochemical Capacitors

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The energy storage devices for wearable electronics require not only excellent electrochemical properties but also mechanical stabilities even under deformations. In order to meet these requirements, we fabricate flexible carbon nanotube (CNT) sheets-based large-scale electrodes decorated with ruthenium (Ru) metal nanoparticles. Our advanced electrochemical capacitors demonstrate enhanced capacitive performance and mechanical robustness even under a severe environment like bending and stretching by electrochemical and structural synergistic effect with Ru and CNT. The facile fabrication process can be easily extended to cost-effective, large-area, and continuous mass production processes that can promote the development of next-generation electronics.

Poster Presentation : **ELEC.P-690**

Electrochemistry

Event Hall FRI 11:00~13:00

Selective electrochemical reductive amination at metal electrode

<u>Taemin Kim</u>, Dong Il Park, Hyo Jae Yoon*, Kyoungsuk Jin[1,*]

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The selective construction of carbon-nitrogen bonds has been considered as one of the central tasks of chemical synthesis, as they are basic structural units that constitute various natural products, pharmaceuticals, and bioactive molecules. For instance, amine functional groups can be found in methyl orange (pH indicator), chlorpheniramine (antihistamine), and adrenaline (hormone). A commonly employed method to prepare amines is reductive amination, which exhibits high chemo-selectivity and is cost-effective. In this study, we demonstrated a new strategy to catalyze the reductive amination process. Imines prepared from aromatic carbonyls and aliphatic amines were further converted into the corresponding amine via electrochemical cathodic reduction. To optimize the catalytic performance, the effects of various electrode materials, solvent/electrolytes, and additives were investigated. We achieved 60-80% Faradaic efficiency at reductant-free conditions. Also, the relationship between applied potential and chemo-selectivity was investigated. We hypothesized that interactions between metal electrodes and imine substrates could enhance the catalytic efficiency of amination. In this regard, a series of electrokinetic studies were conducted to reveal the reaction mechanism. Furthermore, we attempted to expand substrate scopes to stereoselective amination reaction, given that the chiral center of imine induces diastereoselective synthesis based on the reaction mechanism. We believe that our study suggests an eco-friendly electrochemical pathway of reductive amination.

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April 13(Wed)~15(Fri), 2022, ICC JEJU, Korea

Poster Presentation : **ELEC.P-691**

Electrochemistry

Event Hall FRI 11:00~13:00

Highly Selective Electrochemical Oxidation of Furfural to Maleic Acid Using Lead Bismuth Oxide Electrocatalyst

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Biomass is a renewable non-fossil carbon energy source. And furfural, one of the most important platform chemicals, can be synthesized into maleic acid, which has the potential to be a monomer as a bio-derived polymer. Via electrochemical oxidation of furfural to maleic acid, the electrolyte itself acts as an oxidizing agent under ambient conditions. it can be applied in an environmentally friendly way using the sustainable energy derived electricity. It is known that the electrochemical oxidation of furfural to maleic acid through ring opening reaction is favored at high potential under acidic media. Herein, we synthesized lead bismuth oxide alloy electrocatalyst and it shows a highly selective oxidation to maleic acid. From a material screening, the only lead oxide was found to have activity toward Furfural oxidation. Furthermore, by combining lead oxide with other metals, we found that the usage of bismuth element showed enhanced catalytic ability. In the case of conventional lead oxide, it showed a maleic acid yield of 28.7 % and a selectivity of 57.8 %, but when alloyed with the bismuth, a maleic acid yield of 56.7 %, about double fold, and a selectivity of 95 % were shown. We proposed that the oxidation reaction from furfural to maleic acid proceeds via two major steps; first oxidation from furfural to 5-hydroxy-2(5H)-furanone(HFN) and further oxidation to maleic acid. The HFN, an intermediate, was observed to exist in large amounts at the beginning of the reaction. The product chemical distribution suggests that bismuth incorporation promotes the electrochemical oxidation of HFN to maleic acid and prevents overoxidation of maleic acid to CO^2. Through the results, it is expected to be of great help in constructing a catalyst design using bismuth in the electrochemical ring opening reaction or oxidation reaction under high potential.

Poster Presentation : **ELEC.P-692**

Electrochemistry

Event Hall FRI 11:00~13:00

Label-Free MCTA-MWCNT Extended Gate Filed Effect Transistor for Selective Detection of Microcystin-LR in Water Samples

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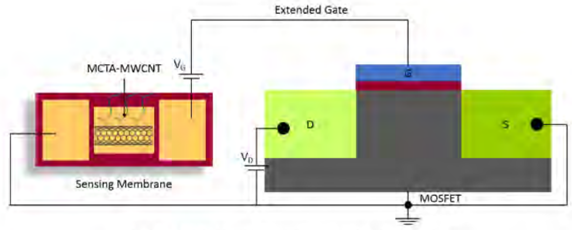
Microcystin-LR (MC-LR) is a cyanotoxin produced by bloom-forming freshwater cyanobacteria. The presence of MC-LR in freshwater bodies has been reported in quite a few areas. Thus, the fabrication of easy-to-use, rapid, robust, and cheap sensors for the detection of MC-LR toxin in drinking water is urgently needed. To address this issue, we have fabricated a label-free biosensor based on aptamer-modified multiwalled carbon nanotube extended gate field-effect transistor (MWCNT-EGFET) for the selective detection of MC-LR. EGFET has two parts MOSFET and sensitive membrane. The only sensitive membrane was exposed to the sample solution. Therefore, the configuration of the EGFET can reduce the cost and influence of the temperature, light, and erosion caused by the sample. A custom-designed DNA oligonucleotide (5-NH_2-C_6-AN_6) was used as MC-LR targeting aptamer (MCTA). MWCNTs were functionalized with MCTA and then stably fixed on the extended Au/SiO_2 electrode (sensitive membrane). The SEM image shows the uniform distribution of MCTA-MWCNT on the Au/SiO_2. Laboratory tap water (TW), filtered tap water from the drinking fountain (FTW), filtered tap water, commercially available mineral water (MW), and filtered water from the Youngju reservoir were used for the experiment. Different concentrations of MC-LR (1-5 ng/mL) caused the change in resistance by a selective interaction with MCTA within 1.5 h. The performance of the aptamer-modified MWCNT-EGFET gave better results than those obtained by liquid chromatography coupled with tandem mass spectroscopy analysis. This study represents the development of an easy-to-use, rapid, robust, and cheap sensor for the selective detection of MC-LR in real-time water samples.



MCTA-MWCNT Modified Extended Gate Field Effect Transistor

Poster Presentation : **ELEC.P-693**

Electrochemistry

Event Hall FRI 11:00~13:00

Atomically Precise $Cl@Ag_8M_6(C\equiv C^tBu)_{12}$(M = Ag, Au) Nanoclusters for Electrochemical CO_2 Reduction to CO

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Electrochemical CO_2 reduction reaction (CO_2RR) is a promising method for transforming CO_2 into value-added chemicals and fuels. Nanostructured catalysts exhibit significantly high CO_2RR activity, but the polydispersity of the size and shape of them makes it difficult to accurately identify the active sites in atom-level. Atomically precise metal nanoclusters (NCs) can be exploited as a powerful model catalysts for identifying the active sites of CO_2RR. In this poster, I present the metal effect of $Cl@Ag_8M_6(C\equiv C^tBu)_{12}$ (M = Ag, Au) NCs on the CO_2RR in a CO_2-fed flow-cell. Both NCs produced CO as a major product. The $Cl@Ag_{14}(C\equiv C^tBu)_{12}$ NC produced CO from overpotential of 54 mV and showed high CO selectivity of 97% at wide potential region. However, $Cl@Ag_8Au_6(C\equiv C^tBu)_{12}$ NC exhibited the gold-doping effect with more positive onset potential (near zero-overpotential) but slightly decreased CO selectivity compared to pure Ag NC. Finally, the studied $Cl@Ag_{14}(C\equiv C^tBu)_{12}$ NC demonstrated highly active CO_2RR activity in a zero-gap CO_2 electrolyzer, producing 385mA/cm^2 of CO current density at a moderate cell potential of 3.0 V.

Poster Presentation : **ELEC.P-694**

Electrochemistry

Event Hall FRI 11:00~13:00

Electrocatalytic Nitric Oxide Generation at Cobalt Oxide electrodes

Sojin Kim, Suyeon Kim, Chanju Won, Hugh I. Kim*, Kyoungsuk Jin*

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Nitric oxide is one of the gaseous messenger molecules that mediate the various biological processes, such as neurotransmission, immune response. The study of the signaling pathway and biological effects of nitric oxide is crucial, although the radical nature of nitric oxide has limited identifying the accurate reaction pathway. Currently, nonspecific nitric oxide-releasing materials have been intensely studied.In this study, we attempted to reveal the biological effects of nitric oxide via an electrochemical platform. Various metal oxide nanocatalysts were synthesized and employed for electrochemical nitrite reduction reactions. One electron reduction of nitric oxide makes the nitric oxide molecules, which competes with the formation of ammonia and water reduction to hydrogen as a side reaction. We investigated 20-30 nm-sized first row transition metal oxide nanoparticles and found out that cobalt oxide nanoparticles are able to selectively produce nitric oxide from nitrite at pH 7 Tyrode's solution with significantly low overpotentials. As a next step, cellular responses were monitored at the designed electrochemical conditions. Chronoamperometry analysis was performed at various cathodic potentials and corresponding cell viability was investigated. As a result, we were able to observe the distinct tendency of cell viability depending on the concentration of nitric oxide molecules which were precisely tuned by electrochemical methods. We believe that our electrochemical system suggests a new direction to study the cellular responses to gaseous messenger molecules.

Poster Presentation : **ELEC.P-695**

Electrochemistry

Event Hall FRI 11:00~13:00

Fabrication of carbon-coated MnO_x-Ni foam electrodes via pyrolysis of α-chitosan and their electrochemical performance

<u>Jaeyoung Hwang</u>*, Kyoung Tae Lee[1]

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[1]*Forest Biomaterials Research center, National Institute of Forest Science, Korea*

Carbon coated MnO_x-Ni foam electrodes were successfully prepared using a combined process of hydrogel reaction followed by high-temperature pyrolysis under air or Ar gas conditions. The prepared samples were analyzed by various characterization tools. To evaluate the performances of the carbon coated MnOx-Ni foam electrodes as supercapacitors, cyclic voltammetry (CV), galvanostatic charge–discharge, electrochemical impedance spectroscopy (EIS) and cycle stability were also carried out. The carbon coated MnO_x-Ni foam electrodes displayed supercapacitive behavior in 1.0 M KOH with a high specific capacitance value of 354.6 Fg^{-1} at 10 mV s^{-1}. The electrode also exhibited remarkable cycle stability. This research provides a valuable and effective approach to enhance the performance of materials applied as supercapacitors.

Poster Presentation : **ELEC.P-696**
Electrochemistry
Event Hall FRI 11:00~13:00

Size Effect of $LiNiO_2$ in Lithium-Ion Batteries

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High nickel layered oxides are attractive cathode materials that can achieve high energy density in lithium-ion batteries (LIBs). Many researchers have strived to improve the cycling stability and energy density of $LiNiO_2$ (LNO) through another metal mixing, dopping, or coating method. However, the particle size effect of pure LNO during the charging/discharging system has not been fully understood yet. Many computing research results revealed that smaller-particle materials with highly connective interfaces and reduced diffusion paths exhibit higher rate performance and good cycling stability than bulk counterparts. However, our study revealed that the different particle size of LNO has a very different trend in contrast to the computation results because they overlooked the influence of primary particles. In this study, we focus on the impact of the particle size distribution of spherical cathode material on positive electrodes in LIBs. We designed four different particle sizes of $Ni(OH)_2$ by controlling pH, time, and agitation speed. When the other conditions were the same except for the particle size, we were able to explore how the grain size, Li off-stoichiometry ($Li_{1-z}Ni_{1+z}O_2$), and activation energy affect the battery performance. Through size comparison, a better understanding of the influence of particle size distribution was obtained, which would be an important basis to engineer electrodes for higher C-rate capability, higher performance, and better stability during battery cycling.

Poster Presentation : **ELEC.P-697**

Electrochemistry

Event Hall FRI 11:00~13:00

Effect of electrolyte cations on Electrochemical Behavior of Electrodeposited Prussian Blue

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Prussian blue (KFeIII [FeII(CN)6]3, PB) the representative active material in the electrochromic devices (ECDs), is known to be sensitive to the type of the counter cation during the redox process due to the cubic lattice channel of PB. The color change of PB thin films occurs upon the intercalation/deintercaltion of counter cations into the lattice channel of PB structure by applied voltage or current. Thus, the electrolyte used in ECDs is to provide counter cations to maintain the electrical neutrality of the PB thin films. Here, we investigated the electrochemical behaviour of the PB thin film under various electrolyte conditions, including Li+, Na+, and K+ cations. The electrochromic decomposition rate of PB decreases sequentially in the order of Li+, Na+ and K+ counter cations in 0.5 M ionic compounds acting as electrolyte solutions. Thus, hydrated Li+ cations (2.37 Å), larger in size than PB lattice channels, accelerated the degradation rate of PB. However, hydrated K+ cations (1.25 Å), smaller in size than PB lattice channels, showed good electrochemical behaviour stability of PB. These results are consistent with the order of the charge transfer resistance (Rct) values of RLi > RNa > RK. Therefore, the cation exchange reactions caused by the redox reaction of PB associated with the molecular recognition of alkali cations in the PB cubic lattice structure are an important factor affecting the electrochromic properties of PB.

Poster Presentation : **ELEC.P-698**

Electrochemistry

Event Hall FRI 11:00~13:00

Flexible and Transparent Electrochemical Sensor for H_2O_2 in Cancer Cell using Platinum Nanoparticle modified Single-walled Carbon Nanotube

Tae Hyun Kim*, Da Eun Oh[1], Hyunju Cho[2]

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One of the active oxygen species (ROS), hydrogen peroxide (H_2O_2), plays an important role in pathological and physiological processes such as cell proliferation, apoptosis, response to chronic diseases, and intracellular signaling. Especially, cancer cells with excessive levels of H_2O_2 are likely to develop into cancer cells as proteins, lipids, and DNA in cells are damaged. Therefore, H_2O_2 can be used as a biomarker to evaluate the difference between oxidative stress capacity and cancer cell detection of various cells, and many researchers have developed various methods of detecting H_2O_2 released from living cells. In this study, we report the transparent and flexible electrochemical sensing platform using platinum nanoparticle (PtNP) modified single-walled carbon nanotube (swCNT) network electrodes for H_2O_2 in cancer cell. Under the optimized conditions, the proposed biosensor demonstrated impressive electrochemical sensing performances to H_2O_2 including wide linear range from 5 μM to 1 mM, and low detection limit of 4.21 μM (S/N = 3) by using the amperometric response. In addition, the proposed sensor exhibited useful performance in the real-time monitoring of H_2O_2 released from living HeLa cancer cell lines. Finally, due to the excellent flexibility and biocompatibility of the PtNP-swCNT film, HeLa cells can be cultured directly on biosensors, and it has been realized that H_2O_2 emission from cells was monitored in real time without signal reduction even when the film was bent.

Poster Presentation : **ELEC.P-699**

Electrochemistry

Event Hall FRI 11:00~13:00

Flexible and Transparent Electrochemical Sensor for H_2O_2 in Cancer Cell using Platinum Nanoparticle modified Single-walled Carbon Nanotube

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One of the active oxygen species (ROS), hydrogen peroxide (H_2O_2), plays an important role in pathological and physiological processes such as cell proliferation, apoptosis, response to chronic diseases, and intracellular signaling. Especially, cancer cells with excessive levels of H_2O_2 are likely to develop into cancer cells as proteins, lipids, and DNA in cells are damaged. Therefore, H_2O_2 can be used as a biomarker to evaluate the difference between oxidative stress capacity and cancer cell detection of various cells, and many researchers have developed various methods of detecting H_2O_2 released from living cells. In this study, we report the transparent and flexible electrochemical sensing platform using platinum nanoparticle (PtNP) modified single-walled carbon nanotube (swCNT) network electrodes for H_2O_2 in cancer cell. Under the optimized conditions, the proposed biosensor demonstrated impressive electrochemical sensing performances to H_2O_2 including wide linear range from 5 μM to 1 mM, and low detection limit of 4.21 μM (S/N = 3) by using the amperometric response. In addition, the proposed sensor exhibited useful performance in the real-time monitoring of H_2O_2 released from living HeLa cancer cell lines. Finally, due to the excellent flexibility and biocompatibility of the PtNP-swCNT film, HeLa cells can be cultured directly on biosensors, and it has been realized that H_2O_2 emission from cells was monitored in real time without signal reduction even when the film was bent.

Poster Presentation : **ELEC.P-700**

Electrochemistry

Event Hall FRI 11:00~13:00

Simultaneous Detection of Dopamine, Ascorbic Acid, and Uric Acid with PEDOT/Graphene Quantum Dots-modified electrode

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Herein, we propose an electrochemical sensor for the simultaneous and individual detection of dopamine (DA), ascorbic acid (AA), and uric acid (UA) by poly(3,4-ethylenedioxythiophene) (PEDOT)/graphene quantum dots (GQD)-modified electrode. The PEDOT/GQD modified electrode was prepared by subjecting a mixed solution of EDOT and Li-GQD to cyclic voltammetry (CV) with an applied potential range from −0.5 to 1.7 V for 30 cycles at a scan rate of 100 mV s^{-1}. The Li-GQD during electropolymerization of PEDOT acts serve as an anionic dopant to induce a conformational change of PEDOT to the quinoid structure. This led to the formation of the PEDOT/GQD with expanded-coil polymeric chains which increases not only intra electron transfer among PEDOT chains but also interfacial charge transfer between the aromatic moieties of target molecules and that of PEDOT through π–π interaction. The modified electrode was characterized using Raman spectroscopy, scanning electron microscope, and transmission electron microscope, photoluminescence spectra. We could observe three well-resolved peaks in the oxidation of DA, AA, and UA by differential pulse voltammetry. The resulting electrode showed the simultaneous and individual determination of AA, UA, and DA with low LODs and wide dynamic ranges. In addition, the proposed sensor exhibited excellent advantages such as high sensitivity, high selectivity, good reproducibility, and stability.

Poster Presentation : **ELEC.P-701**

Electrochemistry

Event Hall FRI 11:00~13:00

Flexible and Transparent Electrochemical Sensor for H_2O_2 in Cancer Cell using Platinum Nanoparticle modified Single-walled Carbon Nanotube

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One of the active oxygen species (ROS), hydrogen peroxide (H_2O_2), plays an important role in pathological and physiological processes such as cell proliferation, apoptosis, response to chronic diseases, and intracellular signaling. Especially, cancer cells with excessive levels of H_2O_2 are likely to develop into cancer cells as proteins, lipids, and DNA in cells are damaged. Therefore, H_2O_2 can be used as a biomarker to evaluate the difference between oxidative stress capacity and cancer cell detection of various cells, and many researchers have developed various methods of detecting H_2O_2 released from living cells. In this study, we report the transparent and flexible electrochemical sensing platform using platinum nanoparticle (PtNP) modified single-walled carbon nanotube (swCNT) network electrodes for H_2O_2 in cancer cell. Under the optimized conditions, the proposed biosensor demonstrated impressive electrochemical sensing performances to H_2O_2 including wide linear range from 5 μM to 1 mM, and low detection limit of 4.21 μM (S/N = 3) by using the amperometric response. In addition, the proposed sensor exhibited useful performance in the real-time monitoring of H_2O_2 released from living HeLa cancer cell lines. Finally, due to the excellent flexibility and biocompatibility of the PtNP-swCNT film, HeLa cells can be cultured directly on biosensors, and it has been realized that H_2O_2 emission from cells was monitored in real time without signal reduction even when the film was bent.

Poster Presentation : **ELEC.P-702**

Electrochemistry

Event Hall FRI 11:00~13:00

Anodized GCE coated on the thionine linked ferrocene dicarboxylic acid for oxidation of dopamine and reduction of H2O2

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A novel dual mediator-type material was prepared by covalently connecting two redox centres Thionine (TH) and Ferrocene dicarboxylic acid (FcDA) was coupled through the amide linkage with help of (N-3-Dimethylaminopropyl)- N′-ethyl carbodiimide hydrochloride (EDC·HCl) and N-Hydroxy benzotriazole (HOBt) as cross-linkers. The electroanalytical measurements and surface characterization of the Thionine linked Ferrocene dicarboxylic acid coated glassy carbon electrode (TH/FcDA/GCE) were studied. TH has used for the electrocatalytic reduction of H2O2 at negative potential side (-0.3 V) and the obtained linear concentration range of 1.5 to 60 μM with LOD of (S/N=3) 0.05 μM and sensitivity of 100.76 μA/μM/cm2, while FcDA was applied for the electrocatalytic oxidation of dopamine (DA) at positive potential side (0.17 V) in the concentration range from 0.3 to 230 μM with LOD of 0.009 μM and sensitivity of 80.22 μA/μM/cm2. The practical utility of the TH/FcDA/GCE was tested for the DA in diluted human urine samples and H2O2 in different milk samples was studied and obtained good recovery results.Keywords: Thionine, Ferrocene dicarboxylic acid, Dopamine, H2O2, Urine samples, Milk samples

Poster Presentation : **ELEC.P-703**

Electrochemistry

Event Hall FRI 11:00~13:00

Dicationic Heteroaryl Pyridinium As a Highly Stable, Soluble, and Crossover-Resistant Anolyte for Nonaqueous Redox Flow Batteries.

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We show the systematic design strategies for pyridinium-based organic redox molecule to enhance the its stability and solubility and suppress the crossover rate for NRFB. A benzo[*d*]thiazole ring, which provides an electron-withdrawing effect, was introduced at the C4 position of pyridinium core by C-H arylation. The addition of the π-conjugation system to the pyridinium redox core was key to enhance chemical and electrochemical stability, resulting in negatively low redox potential of -1.19 ~ 1.21 V vs. Fc/Fc^+. The solubility of pyridinium derivatives was significantly enhanced from 0.26 M to 1.00 M in acetonitrile by simple anion exchange from tetrafluoroborate (BF_4^-) or hexafluorophosphate (PF_6^-) anion to bis(trifluoromethanesulfonyl)imide ($TFSI^-$) anion. Moreover, exchanging the functional group on N of pyridinium from methyl group to cationic 3-(trimethylammonio)propyl (TMAP) group suppressed the crossover rate with an anion-exchange membrane in the NRFB. 4-(benzo[*d*]thaizol-2-yl)-1-(3-(trimethylammonio)propyl)pyridin-1-ium (**TMAP-BTP**) led to electrochemical stability in symmetric cell, showing a capacity decay rate of 0.0083% per cycle. Contrary to the results of only 60% capacity retention after 100 cycle in full cell with 4-(benzo[*d*]thaizol-2-yl)-1-methylpyridin-1-ium (**BTP**) as negolyte, in the case of full cell with **TMAP-BTP** as negolyte, the capacity retention was significantly increased, showing 89.8 % after 100 cycle, which is ~0.08% capacity decay rate per cycle. (**Figure 1**)

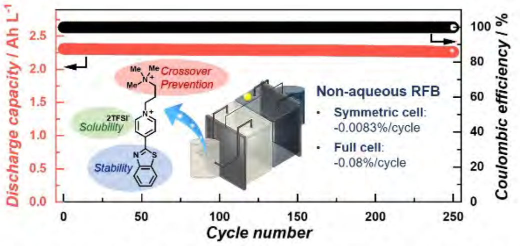

Figure 1. Designed molecular structure of anolyte material and its redox flow battery performances.

Poster Presentation : **ELEC.P-704**

Electrochemistry

Event Hall FRI 11:00~13:00

Simultaneous Detection of Dopamine, Ascorbic Acid, and Uric Acid with PEDOT/Graphene Quantum Dots-modified electrode

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Herein, we propose an electrochemical sensor for the simultaneous and individual detection of dopamine (DA), ascorbic acid (AA), and uric acid (UA) by poly(3,4-ethylenedioxythiophene) (PEDOT)/graphene quantum dots (GQD)-modified electrode. The PEDOT/GQD modified electrode was prepared by subjecting a mixed solution of EDOT and Li-GQD to cyclic voltammetry (CV) with an applied potential range from −0.5 to 1.7 V for 30 cycles at a scan rate of 100 mV s^{-1}. The Li-GQD during electropolymerization of PEDOT acts serve as an anionic dopant to induce a conformational change of PEDOT to the quinoid structure. This led to the formation of the PEDOT/GQD with expanded-coil polymeric chains which increases not only intra electron transfer among PEDOT chains but also interfacial charge transfer between the aromatic moieties of target molecules and that of PEDOT through π–π interaction. The modified electrode was characterized using Raman spectroscopy, scanning electron microscope, and transmission electron microscope, photoluminescence spectra. We could observe three well-resolved peaks in the oxidation of DA, AA, and UA by differential pulse voltammetry. The resulting electrode showed the simultaneous and individual determination of AA, UA, and DA with low LODs and wide dynamic ranges. In addition, the proposed sensor exhibited excellent advantages such as high sensitivity, high selectivity, good reproducibility, and stability.

Poster Presentation : **ELEC.P-705**

Electrochemistry

Event Hall FRI 11:00~13:00

Highly stable aqueous zinc ion battery enabled by Zn deposited flexible carbon cloth anode

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The thermal runways have been a long-standing safety subject hindering the development of high-energy-density batteries. The zinc-ion battery (ZIB) is a past two-century technology but has currently paid attention due to the possibility of switching from primary to rechargeable ZIBs. Nowadays, the ZIBs using a mild aqueous electrolyte are considered one of the chief auspicious candidates for portable electronics applications and energy storage systems (ESS). The nontoxicity, low price, and abundance of zinc than that of other metals (lithium, sodium, and potassium) make it a very attractive candidate for an aqueous metal-ion battery. In addition, the Zn metal has a high theoretical volumetric and gravimetric capacity of 5855 mAh/cm$_{-2}$

Poster Presentation : **ELEC.P-706**

Electrochemistry

Event Hall FRI 11:00~13:00

tert-Butyl alcohol mediated non-hydrolytic synthesis of pre-passivated SnO_2 nanocrystals for perovskite solar cells

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In a typical perovskite solar cell (PSC) structure in which a perovskite layer is sandwiched between a hole transport layer (HTL) and an electron transport layer (ETL), ETL plays an important role in realizing high-efficiency PSCs by extracting and transporting photogenerated electrons. Recently, tin oxide (SnO_2) has attracted growing attention as an ETL material due to its good optical transparency, deep conduction band and high electron mobility. However, SnO_2 surface passivation is inevitable to suppress non-radiative recombination caused by intrinsic defects in the surface. Especially, chlorine (Cl) passivation has been reported to effectively reduce the defects related to Sn dangling bonds. In addition, non-hydrolytic synthesis using an organic solvent has the advantage of high crystallinity and low temperature process compared to the conventional hydrolytic synthesis. In the case of titanium dioxide, it was reported that Cl-passivated colloidal nanoparticles were successfully synthesized through benzyl alcohol (BzOH)-mediated non-hydrolytic route. However, we found that the BzOH-mediated synthetic method was not that effective for synthesizing Cl-passivated SnO_2 colloidal nanoparticles. Instead, in this work, we demonstrated that the synthesis and Cl-passivation of SnO_2 colloidal nanoparticles were significantly more effective when *tert*-butyl alcohol (*t*-BuOH) was used. The PSC fabricated using the *t*-BuOH-mediated SnO_2-based ETL exhibited improved device efficiency, better reproducibility and longer device stability.

Poster Presentation : **ELEC.P-707**

Electrochemistry

Event Hall FRI 11:00~13:00

A serotonin selective voltammetric sensor comprised of DNA and carbon nanotubes composites

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In this work, a biosensor based on modifying positively charged poly(diallyldimethylammonium)-wrapped oxidized single-walled carbon nanotubes (PDDA-oSWCNTs) layer and negatively charged serotonin (5-HT)-specific aptamer layer onto the gold nanoparticles deposited carbon electrode was fabricated for the selective detection of serotonin. This developed biosensor showed linear detection ranges of 50-500 nM with a limit of detection of 2 nM in buffer solution. The biosensor was also applied to analyze the serotonin concentrations in clinical serum samples.

Poster Presentation : **ELEC.P-708**

Electrochemistry

Event Hall FRI 11:00~13:00

Well-designed porous iron-molybdenum oxynitride as electrocatalyst for water electrolysis

Yuanzhe Piao

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Water electrolysis has aroused extensive research efforts due to its potential applications of sewage disposal, microorganism treatment and direct electrolysis for large-scale hydrogen production. In this presentation, I will review our recent progress in the preparation of various electrocatalysts for water electrolysis[1-4]. In search of inexpensive and efficient electrocatalyst for water electrolysis, three strategies to bring out the full potential of the most earth abundant transition metal, iron, are explored: morphology control, secondary metal incorporation, and nitrogen doping.[2] An ultrafast microwave-assisted synthesis of FeMo-MIL-88B followed by self-templated calcination via soft-urea path is developed. The transformed 3D rod-shaped porous iron-molybdenum oxynitride (FeMoON) presents outstanding electrocatalytic performances in hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and overall water splitting. The FeMoON electrode affords high current densities of 850 mA-1 at an over- potential of merely 364 mV for OER and 750 mA-1 at an overpotential of 400 mV for HER. The overall water-splitting demeanor surpasses that of commercial noble metal pair in high current densities and shows potential for long-term stability.[1] Dongjin Ko, Xuanzhen Jin, Kwang-dong Seong, Bingyi Yan, Hua Chai, Jong Min Kim, Minsik Hwang, Juhyung Choi, Wang Zhang*, Yuanzhe Piao*, Few-layered MoS_2 Vertically Aligned on 3D Interconnected Porous Carbon Nanosheets for Hydrogen Evolution, Applied Catalysis B: Environmental, 2019, 248, 357-365.[2] Yejung Choi, Tianyu Chen, Dongwon Kim, Sang Gu Ji, Hwichan Hong, Lulu Lyu, Myeongseok Jang, Yuanzhe Piao*, Transformation of microwave synthesized highly uniform FeMo-MIL-88B nanorod to oxynitride derivate for overall water splitting reaction, Applied Materials Today, 2021, 24, 101093. [3] Juhyung Choi, Daekyu Kim, Weiran Zheng, Bingyi Yan, Yong Li, Lawrence Yoon Suk Lee,* Yuanzhe Piao*, Interface Engineered $NiFe_2O_{4-x}/NiMoO_4$ Nanowire Arrays for Electrochemical Oxygen Evolution, Applied Catalysis B: Environmental. 2021, 286, 119857. [4] Liwei Lin, Shuqing Piao, Yejung Choi, Lulu Lyu, Hwichan Hong, Dohyeong Kim, Jeongyeon Lee,* Wang Zhang,* Yuanzhe Piao,* Nanostructured

Transition Metal Nitrides as Emerging Electrocatalysts for Water Electrolysis: Status and Challenges, EnergyChem, 2022, 4, 100072.

Poster Presentation : **ELEC.P-709**

Electrochemistry

Event Hall FRI 11:00~13:00

Homogeneously dispersed metal single atoms on graphene for hydrogen peroxide production

Dasol Jeong, Jieun Yang[1,*], Hyeon Suk Shin[2,*]

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Metal-nitrogen-carbon (M-N-C) materials are regarded as promising non-noble metal single atomic electrocatalysts. In particular, the Co-N-C on carbon support can be an electrochemically active site for H2O2 production. However, since the synthetic method of Co-N-C on carbon support takes place at a high temperature, it results in a non-uniformly entangled structure of carbon and metal atoms. Thus, it is hard to identify the active site of Co-N-C catalysts and determine the intrinsic catalytic activity. Herein, we show the synthesis of the well-dispersed Co-N-C on the single-layer graphene by using Cobalt phthalocyanine (CoPc). Since CoPc has a planar structure, it can be homogeneously coated on graphene with van der waals interaction between CoPc and graphene. The CoPc anchored on graphene shows the enhanced activity for ORR. We can confirm the role of Co-N-C for ORR from the homogeneously dispersed CoPc. This work presents a new perspective in determining the active sites of Co-N-C.

Poster Presentation : **ELEC.P-710**

Electrochemistry

Event Hall FRI 11:00~13:00

Stabilization of metastable phase WS_2 quantum dots via Re doping for enhanced HER performance

HoonJu Lee, Hyeon Suk Shin[1,*]

Energy Engineering, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Although layered transition metal dichalcogenide (TMD) nanosheets have attracted great attention due to their unique properties, it still remains challenge to develop a facile strategy for the precise control of the lateral size. Moreover, metallic phase of TMD monolayers have been demonstrated as promising electrocatalysts for hydrogen evolution reaction (HER) induced by the high intrinsic conductivity, however, the key challenges to maximize the catalytic activity are achieving the metallic phase with high concentration and increasing the density of the active sites. In this study, we demonstrate a solution-based synthetic protocol to prepare WS_2 quantum dots (QD) which possess extremely small lateral dimensions facilitating expose of edge sites, and WS_2 doped with rhenium (Re). The presence of Re converts the material to stable distorted tetragonal structure (93% phase purity) that shows enhanced HER activity (with Tafel slope of 44 mV/dec and 158 mV at a current density of 10 mA/cm^2) as compared to most of the WS_2-based catalyst reported in the literature which including the normally inert basal planes of 2D layer of WS_2. More importantly, this new alloy catalyst shows high HER catalytic activity and stability. The role of Re is to stabilize the 1T’ phase structure, while catalysis occurs primarily in local W-rich 1T’ phase configurations, where the HER catalytic activity is very close to that in Pt. The study provides a new strategy to improve the overall HER performance of WS_2-based materials via chemical doping.

Poster Presentation : **ELEC.P-711**
Electrochemistry
Event Hall FRI 11:00~13:00

Effects of bases and TEMPO on electrochemical dehydrogenation of heterocyclic compound 1,2,3,4-tetrahydroquinaldine

Aeri Chu, Joohoon Kim*

Department of Chemistry, Kyung Hee University, Korea

As a liquid organic hydrogen carriers (LOHC), nitrogen-containing heterocyclic compounds attract increasing attention because their dehydrogenation process is thermodynamically more favorable than homocyclic compounds. Electrochemical dehydrogenation of such heterocyclic compounds would be also attractive if it could be applied for direct organic fuel cells under relatively mild conditions. In this study, we report the effects of base and TEMPO on the electrochemical dehydrogenation of 1,2,3,4-tetrahydroquinaldine (THQ). We also pursue efficient and selective electrochemical dehydrogenation of THQ under appropriate base conditions with TEMPO.

Poster Presentation : **ELEC.P-712**

Electrochemistry

Event Hall FRI 11:00~13:00

Electrochemiluminescence on hematite(α-Fe_2O_3) photoanodes prepared by hydrothermal and electrodeposition processes.

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Hematite(α-Fe_2O_3) is an n-type semiconductor, which has bandgap of 1.9 to 2.2 eV. It is a promising photoanode material for photoelectrochemistry(PEC) due to its stability in aqueous solution and its ability for visible light absorption. In this study, we compared photoelectrochemical features of hematite photoanodes prepared on fluorine-doped tin oxide(FTO) by hydrothermal and electrodeposition processes. Specifically, we compared electrochemiluminescence features of the hematite photoanodes prepared by the different processes; hydrothermal and electrodeposition.

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Poster Presentation : **ELEC.P-713**

Electrochemistry

Event Hall FRI 11:00~13:00

Porous Mo-based catalyst as an efficient electrochemical nitrogen reduction reaction

YunHwi Seong, Shinyoung Kweon, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Ammonia (NH_3) is one of the increasing future energy resources worldwide for the production of industrial chemicals such as plastics, pharmaceuticals, agricultural fertilizers, textiles and other industrial raw materials. At present, Haber-Bosch process for industrial-scale NH_3 production requires harsh reaction conditions, 300℃-500℃ and 200-300 atm, because N_2 triple bond is a chemically very stable gas molecule and has a high bond energy (940.95 kJ/mol). Thus, the process leads to excessive consumption of non-renewable resources as well as the increase of carbon dioxide emissions. To address these issues, an ideal technology is desired to develop a green and economical ammonia synthesis method such as electrochemical N_2 reduction to NH_3 (NRR). In this presentation, we report a novel strategy to synthesize porous Mo-based nanostructures as a high-efficiency alternative catalyst for electrochemical NRR. Boron and sulfur has been explored as p-block catalysts to improved NH_3 yield and faradaic efficiency (FE) for NRR. A dual-layer electrode is prepared by spraying the catalysts on carbon cloth, serving as the working electrode for nitrogen reduction to ammonia in a H-type cell. The catalytic activity for NRR was investigated using conventional electrochemical techniques and spectrophotometry. The as-synthesized porous Mo-based catalysts can achieve high NH_3 yield rate and FE.

Poster Presentation : **ELEC.P-714**

Electrochemistry

Event Hall FRI 11:00~13:00

Vat dyes as a cost-effective organic cathode material for sustainable secondary batteries

Jinyoung Lee, Jong-Jin Park, Ji Eon Kwon*

Functional Composite Materials Research Center, Korea Institute of Science and Technology, Korea

As the demand for wearable and mobile electronic devices has recently increased, rechargeable lithium-ion batteries (LIBs) have gained tremendous interests. However, since conventional electrode materials in LIBs are obtained through mining, a lack and an uneven geometric distribution of the resources have steeply raised their price. Therefore, it is essential to develop new electrode materials consisting of more abundant elements for next-generation batteries. Here, we report Vat Blue (VB) dyes as a low-cost organic cathode material in batteries. Because the VBs bearing redox-active conjugated carbonyl groups have already been commercialized in dyeing applications, it also has the great potential for a low-cost electrode material. To improve processability of VBs, we introduced thermally cleavable tert-butyloxycarbonyl (t-BOC) groups. In the electrode fabrication process, highly soluble t-Boc-VBs formed homogeneous films with conductive carbon additives and PVDF binder. Subsequently, the drying process spontaneously removed the t-Boc group from the VB molecules to form insoluble active materials in the electrode. Due to low solubility, the electrode showed stable cyclability in coin cells.

Poster Presentation : **ELEC.P-715**

Electrochemistry

Event Hall FRI 11:00~13:00

Counter anion effect on the electrochemical properties of Viologen electrodes in lithium-organic batteries

Yunho Cho, Jong-Jin Park, Ji Eon Kwon*

Functional Composite Materials Research Center, Korea Institute of Science and Technology, Korea

The demand for battery has rapidly increased due to the growth of electromobility industry. As the research trends move toward developing more sustainable electrode materials such as organic molecules, viologens have been drawing great attention. To date, significant progress has already been made in aqueous organic redox flow batteries (AORFBs); however, viologens have poorly been investigated as electrode materials in the stationary-type (i.e., solid-type electrodes) batteries. Furthermore, despite the fact that the counter anions can significantly influence the electrochemical properties of the viologens as a charge-carrier, systematic studies are scarcely reported, so far. In this study, we investigated relationship between the electrochemical property of ethyl viologen and types of its counter anion, including chloride, bromide, iodide, bis(Trifluoromethanesulfonyl)imide (TFSI), hexafluorophosphate, and perchlorate. The redox mechanism and electrode performances depending on the types of counter anions and electrolyte salts were also systematically investigated to provide a deeper insight into designing viologen-based electrode materials.

Poster Presentation : **ELEC.P-716**

Electrochemistry

Event Hall FRI 11:00~13:00

Study on Gradually Oxidizing Phenomena of Single Nickel nanoparticle for Urea Oxidation by Electrocatalytic Amplification Method

Ki jun Kim, Seong Jung Kwon[*], Seungyoung Park

Department of Chemistry, Konkuk University, Korea

Nickel (Ni) showed electrocatalytic character for urea oxidation when Ni is oxidized. Electrocatalytic amplification method was used to investigate single Ni nanoparticle (NP)’s electrochemical behavior about urea oxidation. Platinum (Pt) is not good catalyst for urea oxidation, so Pt is appropriate for working electrode. According to Cyclicvoltammetry (CV) results, oxidized Ni showed catalytic current at 0.4 V region. So Ni nanoparticle (NP) collided on Pt electrode surface applied 0.4 V, the transient current signals were showed depending on Ni NP’s oxidation states. To control Ni NP’s oxidation state, Ni NP stock solution was bubbled with Oxygen. At first Ni NP didn’t showed current signal. But as time goes by, the surface of the nickel was oxidized so transient current signals were showed. This amplified signal was observed as staircase signal. The signal's peak height and frequency increase over time after oxygen exposing to Ni NP solution. Through this results, we detected Ni NP's gradually oxidizng affect on urea oxidation via electrocatalytic amplification method.

Poster Presentation : **ELEC.P-717**

Electrochemistry

Event Hall FRI 11:00~13:00

Investigation of I- electro-oxidation mechanism at platinum microelectrode

<u>Sehyeok Ki</u>, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

Electro-oxidation of I- is a half redox reaction occuring on the cathode of iodide-based aqueous electrical energy storage system. Therefore, understanding the I- electro-oxidation is important to enhance the performance of the energy storage system. However, the oxidation mechanism is complicated by a formation of metastable iodine films, which inhibit the electrode kinetics of I- oxidation. Because of the complicated reaction mechanism, their formation and effect on the electrode kinetics has been largely unexplored. Here, we investigate the I- electro-oxidation mechanism at platinum microelectrode in the presence of concentrated supporting electrolytes using cyclic voltammetry and chronoamperometry. Surprisingly, cyclic voltammogram shows linear current-voltage relationship and current which far outweighs diffusion-limited value. Also, the cyclic voltammogram clearly shows higher conductance, current and shifted onset of linear current-voltage behavior as the concentration of supporting electrolytes increases. This linear current-voltage behavior could imply a formation of porous iodine structure at platinum electrode surface, which generates the I- ion current.

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Poster Presentation : **ELEC.P-718**

Electrochemistry

Event Hall FRI 11:00~13:00

Redox-Reversible Vitamin-C Confined in Microporous Carbon

Sarah Choi, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

In this article, we fully demonstrated that ascorbic acid can turn to be redox-reversible when it is confined in microporous regimes. Redox-reversibility in an electrochemical reaction coupled with an irreversible chemical process can be enhanced due to kinetic acceleration toward the inverse direction derived from accumulation of redox species in microporous networks. However, the kinetic acceleration in a microporous domain is revealed to have a certain limitation for the enhancement of the redox-reversibility, which is indicative of the important aspect for stabilization of the species undergoing a side product as the other critical factor to achieve the redox-reversibility enhancement.Redox-reversible voltammetric features of ASC in the three different types of buffered solutions with a neutral pH were observed from the electrode composed of microporous carbon, which were not shown from the one with non-porous carbons. The investigated redox-reversible behavior confined in microporous carbon were found to be dependent on both the types of the buffers and pH.The origin of nanoporous confinement of ASC and its enhanced redox-reversibility was rationalized by the MD simulation. From the simulated results, we found a ASC-cluster between H2A and HA- forms inside of a carbon pore, which would be a possible main driving force for its confinement in a microporous carbon regime. In addition, the simulated radial distribution functions gave the evidence that A from a ASC-cluster was less probable to be reacted with a water molecule than its free form. This stabilization of A by its interaction with HA- in the ASC-cluster could lead enhanced redox-reversibility.We demonstrated charge-discharge curves of the electrochemical cell as redox electrolyte in an aqueous ESS.

Poster Presentation : **ELEC.P-719**

Electrochemistry

Event Hall FRI 11:00~13:00

Voltammetric kinetic discrimination of two sequential proton-coupled electron transfers in serotonin oxidation: Electrochemical interrogation of a serotonin intermediate

Jeongmin Yeo, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

An understanding of the electrochemical mechanism involved in serotonin oxidation is critical to the development of accurate sensing applications. Electrochemical signals of a reactive serotonin intermediate can reveal detailed mechanistic information. Here, oxidation of a serotonin radical intermediate, $SH^{\bullet}$, is electrochemically interrogated in a buffered system at a neutral pH by voltammetric kinetic discrimination (VKD). At a low scan rate of 0.02 V/s, the voltammogram showed one oxidation peak that can be attributed to electro-oxidation of serotonin with two proton-coupled electron transfers (PCETs) in the absence of voltammetric resolution. This corresponds to the inherent thermodynamic instability of a reactive serotonin intermediate, leading to potential inversion in two sequential PCETs. However, at a scan rate of 1 V/s, the single voltammetric peak gradually resolved into two, each of which are associated with sequential electro-oxidation of serotonin via $1e^{-}$-$1H^{+}$. The peak resolution originated from kinetic discrimination between the first and second PCET in serotonin oxidation; the first PCET step is Nernstian, while the second is electrochemically irreversible. The observed VKD in electro-oxidation of serotonin can be explained by voltammetric simulations.

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Poster Presentation : **ELEC.P-720**

Electrochemistry

Event Hall FRI 11:00~13:00

Electrode interface characterization by electrochemical redox probe in water-in-salt electrolytes

Cheolmin Park, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

Water-in-salt electrolytes (WiSEs) have attracted attention in the effort to replace organic electrolytes. The principle of making this electrolyte is that the solvation structure changes when a very highly soluble solute is dissolved in water. Previous studies have focused on the bulk properties of electrolytes. So, there have been many reports of applications to battery using such properties. However, there are few studies about interfacial properties between the electrode and the solution in this electrolytes. In this work, we reported the interface characterization on Pt in WiSEs by redox probe, H2/H+ redox reaction. We observed the reversible cyclic voltammogram (CV) of H2/H+ redox reaction in WiSEs. This result means that hydrogen can be stable in aqueous phase. We associated this result with interfacial property which can be formed specially in WiSEs. We think that there is a heterogeneous phase in which a region that can stabilize non-polar molecules on working electrode.

Poster Presentation : **ELEC.P-721**

Electrochemistry

Event Hall FRI 11:00~13:00

Stochastic Particle Approach Electrochemistry (SPAE): Estimating Size, Drift Velocity, and Electric Force of Insulating Particles

Heejung Chung, Jinho Chang[1,*]

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Stochastic particle impact electrochemistry (SPIE) is considered one of the most important electro-analytical methods to understand the physicochemical properties of single entities. SPIE of individual insulating particles (IPs) has been particularly crucial for analyses of bioparticles. In this article, we introduce stochastic particle approach electrochemistry (SPAE) for electrochemical analyses of IPs, which is the advanced version of SPIE; SPAE is analogous to SPIE but focuses on deciphering a sudden current drop (SCD) by an IP-approach toward the edge of an ultramicroelectrode (UME). Polystyrene particles (PSPs) with and without different surface functionalities (−COOH and – NH3) as well as fixed human platelets (F-HPs) were used as model IPs. From theory based on finite element analysis, a sudden current drop (SCD) induced by an IP during electro-oxidation (or reduction) of a redox mediator on a UME can represent the rapid approach of an IP toward an edge of a UME, where a strong electric field is generated. It is also found that the amount of current drop, idrop, of an SCD depends strongly on both the size of an IP and the concentration of redox electrolyte. From simulations based on the SPAE model that fit the experimentally obtained SCDs of three types of PSPs or F-HP dispersed in solutions with two redox electrolytes, their size distribution histograms are estimated, from which their average radii determined by SPAE are compared to those from scanning electron microscopic images. In addition, the drift velocity and corresponding electric force of the PSPs and F-HPs during their approach toward an edge of a Pt UME are estimated, which cannot be addressed currently with SPIE.

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Poster Presentation : **ELEC.P-722**

Electrochemistry

Event Hall FRI 11:00~13:00

Attachable micropseudocapacitors based on highly swollen femtosecond-laser-induced-graphene electrodes

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The rapid growth of miniaturized wearable and portable electronics has increased the demand for power sources that are sufficiently compact and can be directly integrated with them. Microsupercapacitors (MSCs) are recognized as the potential power supply devices due to their high power density, long operating lifetime and excellent rate performance. In this regard, MSCs with unique in-plane, interdigitated electrode design provide flexibility and ease of integration with wearable and portable electronics. However, MSCs are still limited in terms of design flexibility, scalability, reusability, and compatibility with basic components of wearable devices, such as textile, paper and plastic, etc. In this study, we report a high-performance sticker-type flexible microsupercapacitor using highly swollen reduced-graphene-oxide electrodes fabricated by a femtosecond-pulse laser to promote full active-site and durability of the electrodes.

Poster Presentation : **ELEC.P-723**

Electrochemistry

Event Hall FRI 11:00~13:00

Crystal structure and phase-transition of a new sodium-ion conducting material $NaTa_2PO_8$ prepared via the Li^+/Na^+ ion-exchange reaction of $LiTa_2PO_8$

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Ion exchange reaction is a promising method to explore metastable compounds that could not be synthesized by the conventional high-temperature solid-phase reactions. Herein, a new sodium tantalum phosphate. $NaTa_2PO_8$ was synthesized via the Li^+/Na^+ ion-exchange reaction of the parent compound, $LiTa_2PO_8$ in molten $NaNO_3$ medium. $NaTa_2PO_8$ underwent an irreversible phase transition from the low-(α-$NaTa_2PO_8$) to the high-temperature polymorph(β-$NaTa_2PO_8$) at approximately 1000 ℃. The crystal structures were solved using an ab initio structural determination method based on synchrotron X-ray powder diffraction data. The α-$NaTa_2PO_8$ presented an orthorhombic structure, closely related to that of the parent $LiTa_2PO_8$ structure. In contrast, the β-$NaTa_2PO_8$ was found to adopt a monoclinic structure, belonging to a family of monophosphate tungsten bronzes with with pentagonal tunnels. The ionic conductivities of α-$NaTa_2PO_8$ ($\sigma = 5 \times 10^{-5}$ S/cm at 309 ℃) and β-$NaTa_2PO_8$ ($\sigma = 2 \times 10^{-7}$ S/cm at 300 ℃) exhibited Arrhenius behavior with activation energies of 0.49 and 0.79 eV, respectively. Bond valence energy landscape (BVEL) calculations indicated that a three-dimensional (3D) conduction pathway is formed in α-$NaTa_2PO_8$ structure, while the conduction pathway in β-$NaTa_2PO_8$ shows a two-dimensional (2D) character.

Poster Presentation : **ELEC.P-724**

Electrochemistry

Event Hall FRI 11:00~13:00

MoS2-graphene composite with phase controlled MoS2 and its application for lithium ion battery

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Electric vehicles and various electronic devices require a battery with a higher capacity, and it is essential to develop an anode material with a higher capacity. Therefore, anode materials using Si are in the spotlight, but Si has a higher capacity (~4200mAh/g) than conventional graphite materials, but there is a problem of volume expansion when the cycle is performed.Transition metal dichalgogenides materials are attracting a lot of attention because of their structural properties and high storage capacity. The theoretical capacity of MoS2 is known to be 670 mAh/g, making it a promising material for a new LIB anode material. In particular, it is very advantageous to make a single layer of MoS2 because their layered structure is combined with a weak van der walls force. It is typically known to have 1T and 2H structures. The 1T phase of MoS2 has the properties of a conductor and therefore has excellent conductivity as a LIB anode material. 1T structures can be produced when a single layer is made through exfoliation. However, due to its metastable structure, it is easily converted to the 2H phase as the most stable phase. In this study, a composite of MoS2 and graphene was prepared by a chemical exfoliation method, and through this, a stable and high-capacity anode material was realized using the high energy storage capacity of MoS2 and the stability of graphene. In addition, a mixed phase of 1T and 2H structures was generated through the post-treatment process, and it was confirmed that the 1T phase was stably present. The diffusion of Li+ was facilitated by securing wide interface spacing and high conductivity of the 1T phase, and as a result, superior conductivity and high capacity were stably maintained compared to the single-phase material of the 2H structure.

Poster Presentation : **EDU.P-691**

Chemistry Education

Event Hall THU 11:00~13:00

Development of creative quizzes to improve the scientific creativity: Focused on the Chemistry I

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The purpose of this study is to develop creative quizzes to improve the scientific creativity of high school students. The types of creative quizzes were investigated and classified into five categories such as picture arrangement regularity finding type, number or letter arrangement regularity finding type, criminal finding type, logic reasoning and language play type, and stick or matchstick utilization type. Creative quizzes were developed for each sub-unit of the Chemistry I subject under the current 2015 revised curriculum. In each quiz, the elements of creativity required to solve the quiz were specified as fluency, flexibility, unusual thinking, similarity-based thinking, dissimilarity-based thinking, and originality. The creative quizzes developed in this study can be used for the purposes such as arousing interest and curiosity, concentration of attention, and organizing content in various teaching and learning situations, such as the chemistry classes, the mentoring, the educational volunteering, the club activities, and the school events. In addition, the method for developing a quiz was presented so that teachers can develop and utilize creative quizzes for other subjects or contents.

Poster Presentation : **EDU.P-692**

Chemistry Education

Event Hall THU 11:00~13:00

What to Consider in Overseas Educational Voluntary Activity: Focused on Nicaragua

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Korean teachers and professors have been participated in the overseas education voluntary activity for many years. In that activity the participants should consider many things of the foreign country where they work. Among the six factors of the cultural historical activity theory, such things surrounding and thus affecting an activity are classified as the ‘community’ or the ‘rule.’ This study aims to analyze the community and the rule of overseas educational voluntary activity in Nicaragua. There is no high educational fervor in Nicaragua as in Korea. The low educational fervor may be related to the fact that the education is not linked to the success in getting a good job. The society of Nicaragua does not seem to encourage students to study hard. On the contrary the school education is limited strongly. For example, the elementary or secondary school should provide only five classes in a day. The number of the teacher and the school is limited, so there are the two-part schools where students go to school in turns in the morning and in the afternoon. The dreams of the high school or the university students are going abroad to find a good job and make money for their family. The situations of Nicaragua have both the similar part and the different part with Korea in 1970’s or 1980’s. In the overseas activity, the volunteers should be aware of the social, educational, and cultural situation of the foreign country. (This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea (NRF-2018S1A5A2A01036487))

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Poster Presentation : **EDU.P-693**

Chemistry Education

Event Hall THU 11:00~13:00

A Narrative Inquiry on the experience of participating in online overseas educational voluntary activities

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There are an increasing number of cases in which people cannot go abroad due to the Covid-19. People connect with the foreign countries in online to perform the voluntary activities. This study seeks to find out what experiences pre-service teachers have in participating in the online overseas educational voluntary activity. It explores how the socio-cultural situation and the educational variables affect pre-service teachers. Also we try to find out the characteristics of what they experience in the online educational activities compared to the face-to-face situation. We conducted the pre- and post- interviews and surveys with Chungbuk National University students majoring in education who participated in the online volunteer activities in Nepal, Guatemala and Nicaragua, as well as students not majoring in education but taking the teaching profession. Researchers participated in the volunteer activities as the members, performed the participant observation, and conducted the research. The experiences are analyzed by the narrative inquiry method. The members were aware of the poor educational situation of the underdeveloped countries and made more efforts to prepare the classes. They taught the foreign students speaking a language different from their own, and confirmed the importance of the interaction between teachers and students. They also found the joy of the interaction through the lessons even in non-face-to-face situations. They learned that there are many difficulties in conducting the overseas educational voluntary services, and recognized the importance and necessity of the continuous volunteer activities.

Poster Presentation : **EDU.P-694**

Chemistry Education

Event Hall THU 11:00~13:00

Effect of student-driven evaluation on science learning achievement and achievement emotions of middle school students.

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This study attempted to investigate the effect of student-driven evaluation on the science learning achievement and achievement emotions of middle school students. To this end, a student-driven evaluation was conducted after 10 science classes were conducted for middle school students located in Gyeongsangnam-do. After students took the initiative in setting achievement standards and levels, self-evaluation and peer evaluation were applied only to the experimental group (4 classes), and the comparative group (3 classes) conducted teacher-driven evaluation. To examine the effectiveness of student-driven evaluation, academic achievement tests and achievement sentiment tests using national-level achievement evaluation were conducted on both pre-and post-groups. In addition, interviews were conducted with students with significant changes to analyze the effectiveness of student-driven evaluation in depth. Based on these results, I would like to propose a plan to utilize student-driven evaluation to increase students' participation in learning as subjects of learning.

Poster Presentation : **EDU.P-695**

Chemistry Education

Event Hall THU 11:00~13:00

Remote Chemistry Experiment using 6-Axis Robot Arm

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COVID-19 changed the whole lifestyle all over the world. All educational institution turned in-person classes to online classes including experiment classes in university. Most of university are replacing to video-protocol taken by training assistant, however, it lacks a lot of main elements of experiment done by students themselves. In this study, I designed the remote chemistry experiment using a 6-axis robot arm which is operated by students from a distance. The robot arm was connected by TCP/IP communication using 2 computers, one for controlling robot arm directly and the other for students. There are 6 zone and each one is apparatus, preparing sample, reaction, pipetting, post-processing and detection zone. ArUco marker was used to get position of each apparatus differ from experiments. Robot movements are defined as a module that students can use correspondingly. Students can get deeper understanding doing their own experiment instead of using an uniform data.

Poster Presentation : **EDU.P-696**

Chemistry Education

Event Hall THU 11:00~13:00

The Effects of the role assignment on middle school students's collaboration in the Collaborative Problem Solving for Character Competency (CoProC) science classes

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The purpose of this study was to examine the effects of the role assignment on students's collaboration in applying the Collaborative Problem Solving for Character Competency (CoProC) for the purpose of improving character competency in the middle school science classes. The participants of the study were 122 middle school students (four classes). Two classes (62 students) were assigned to the non-role assignment group and the other two classes (60 students) were assigned to the role assigned group. Both groups of students participated in the Collaborative Problem Solving for Character Competency classes for one semester. Four topics were implemented. Data was collected from character competence test (pre- and post-), group discussion voice recordings, and activity worksheets. We analyzed student's collaboration expressed in group discussions and the CoProC activity worksheets to look at the effects of role assignment. For the analysis of collaboration in group discussion, we developed an analytical framework for collaboration.

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Chemistry Education
Event Hall THU 11:00~13:00

Learning the principles of electrochemical cell using the Voltaic cell: Analysis of textbooks from 1'st to 2015 revised curriculum period and probing concepts of students.

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This study analyzed the change of description for the Voltaic cell and principles of electrochemical cell in science and chemistry textbooks used in the course of secondary school from the first to the 2015 revised curriculum period, and probed the concepts of students for the basic phenomena of the Voltaic cell. The learning of principle of electrochemical cell has great attention in curriculum along with the development of technology of the diverse eco-friendly batteries. However, the description for principles of electrochemical cell in science and chemistry textbooks in secondary school has not been changed from first curriculum period. Furthermore, the Voltaic cell has been frequently introduced to explain the electrochemical cell, but it has been reported to have problems in real experiments and show complex phenomena that cannot be explained by the scientific knowledge level of secondary school. Students who have learned the concepts of oxidation, reduction, ionization tendency, electromotive force showed the difficulties predicting and explaining the simple phenomena occurred in the Voltaic cell experiments especially for the "why does the gas evolve at both electrode?, Why can the potential have the values when distilled water is used instead of acidic water?" Based on these analyses, this study suggests the effective learning case of the principle of electrochemical cell using problem finding inquiry of the Voltaic cell.

Poster Presentation : **ENVR.P-698**

Environmental Energy

Event Hall THU 11:00~13:00

Environmentally safe and renewable solar vapor generation device based on Prussian blue nanoparticles immobilized on cellulose nanofibers

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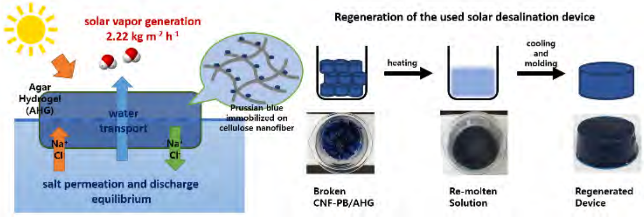
Solar vapor generation devices received a great attention due to their capability to overcome the shortage of fresh water. Although several solar vapor generation devices showing significant evaporation rates have been developed over the past years, there are still remaining problems such as fabrication difficulties and potential environmental hazards. Here, we demonstrate an environmentally safe, renewable and easily manufacturable evaporation device composed by agar hydrogel (AHG) and Prussian blue (PB) nanoparticles immobilized on cellulose nanofiber (CNF). The suggested device shows a high evaporation rate of 2.22 kg/m2h under 1 kW/m-2 illumination thanks to the combined effects of the high water-transport performance of CNF/AHG and the good photothermal ability. The device shows remarkable desalination performance as high as 13.26 kg/m2day in the field test due to the salt-rejection ability of AHG. Furthermore, the used device can be resurrected without decline of the performance through a simple re-fabrication process due to the remarkable stability of CNF-PB and reversible sol-gel transition of AHG. Our results suggest a facile and promising method to environmentally safe, low-cost, renewable, and easily manufacturable solar desalination system, which can be a promising solution to supply quality and quantity of fresh water for basic humanity.



Poster Presentation : **ENVR.P-699**

Environmental Energy

Event Hall THU 11:00~13:00

Evaluation of Electrochemical Characteristics of bifacial modified-TNTs electrodes

Soyoung Yang

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Owing to low cost and high stability, TiO_2 have been extensively studied for several decades for use in water treatment applications such as organic pollutant treatment and heavy metal adsorption. Various modifications have been proposed the surface defects, non-metal doping and metal-deposition to improve their performance. With this in mind, we synthesized modified-TNTs samples via sequential electrochemical processes of anodization and/or cobalt ions via wet adsorption. This performed the electrocatalytic activities for the decomposition of an organic/inorganic substrate and inactivation of E. coli.

Poster Presentation : **ENVR.P-700**

Environmental Energy

Event Hall THU 11:00~13:00

A Role of Ionomers in Catalyst Layers for Electrochemical Reactions of Hydrogen-Based Energy Conversion Devices

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Green hydrogen production is of importance in the upcoming hydrogen economy era. Proton exchange membrane water electrolysis is one of the most important technology to produce the green hydrogen. Hydrogen Fuel cells are common devices for hydrogen utilization. For both devcies, membrane electrode assembly (MEA) has the most important role in all components for fuel cell performance. MEA is consist of membrane and both side of catalyst layer, the catalyst layers were made of electrocatalyst and ionomer by evaporating all solvents in the catalyst inks. Ionomer binder in catalyst layers plays an important role in conducting proton, which wraps electrocatalyst to make unique microstructure for triple phase boundary. The structure of catalyst layer is formed differently according to type of ionomer, which could be make difference performance of catalyst layer. In this study, the effect of side chain length in different of ionomer dispersions on the microstructure of catalyst layers has been investigated: two types of ionomers were used: i) long-side chain ionomer and ii) short-side chain. Prepared catalyst layers were characterized by electrochemical evaluation such as I-V curve, cyclic voltammetry, electrochemical impedance spectroscopy and by physical and microscopic characterization such as porosimetry and scanning electron microscopy.

This research was supported in part by the Hydrogen Energy Innovation Technology Development Program of the National Research Foundation (NRF) funded by the Ministry of Science, ICT & Future Planning(NRF-2019M3E6A1063677).

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Poster Presentation : **ENVR.P-701**
Environmental Energy
Event Hall THU 11:00~13:00

Analysis of metal impurities in carbon-based materials and refining method

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Carbon black (CB), a material consisting of finely divided particles, can be obtained by the partial combustion of heavy petroleum feedstock. The combustion or partial gasification of oil or heavy oil, with the use of air or oxygen and, if appropriate, stem, results in the formation of carbon black which partially contains substantial amounts of metals or metal compounds. Typical metal components are iron, chrome, and nickel, which are present in carbon black. In our study, it relates more particularly to a process for the removal of metals, especially, by treating an aqueous suspension of the carbon black with an acid/base agent suitable for dissolving the metals or their compounds at an elevated high temperature. Therefore, good quality CB’s useful for batteries, sensors, electronic devices, catalysis, among many other higher applications.

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Poster Presentation : **ENVR.P-702**

Environmental Energy

Event Hall THU 11:00~13:00

Preparation and Characterization of Phosphorus-containing Flame Retardants

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Recently, restrictions on the use of halogen flame retardants have resulted in the development of eco-friendly flame retardants, and phosphorus-containing flame retardants are one of the well-known candidates. Among them, organo-phosphorus and phosphorus─nitrogen flame retardants appear to be very effective fire retardants and they produce less toxic moiety and smoke during combustion. The flame retardant's action works either in the condensed phase or the gas phase or in both phases through a physical and/or chemical mechanism. The flame retardant efficiency is also contributed from residual char acting on condensed phase to protect the material from flammable gas, oxygen, and heat. In this study, three types of non-halogen phosphorus-based flame retardants were synthesized and investigated the physical/chemical properties of flame retardants.

Poster Presentation : **ENVR.P-703**

Environmental Energy

Event Hall THU 11:00~13:00

A colorimetric method of dichromate ion detecting probe based on the aggregation of Au Nano star particles

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A sensitive and selective colorimetric sensing assay was developed using flower-shape gold nanoparticles (AuNFPs) for the determination of dichromate ions in aqueous samples. The AuNFPs was synthesized by indicator (ligand) free for dichromate ions and stabilized using PVP. AuNFPs conducts an aggregating reaction to dichromate ions, resulting in a dramatic color change from purple to blue. Therefore, the concentration of dichromate ions in environmental samples can successively quantitate by the naked eye or by UV-Vis spectrometry using the proposed AuNFPs sensor. The optimal conditions such as pH, temperature in solution stimulated to a more rapid color change in the optimized AuNFPs system. The absorption ratios (A800 nm/A575 nm) of the optimized AuNFPs solution exhibited a linear correlation with the dichromate ions with concentrations (y=0.6836x+0.1215, r2=0.9992) and with a limit of detection of 3.03 nM, respectively. This sensor has high property and can selectively detect only dichromate ions.

Poster Presentation : **ENVR.P-704**
Environmental Energy
Event Hall THU 11:00~13:00

Tailoring Supramolecular Structures of Organic Chromophore for Bio-hybrid Hydrogen Evolution System

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Hydrogen evolution system using solar energy is being studied as an attractive approach for sustainable society due to its most abundant resource feature. However, current hydrogen production process is still mostly dependent on photovoltaic and photocatalytic technology based on artificial inorganic or organic semiconductors. This study describes a nature-inspired hydrogen production strategy which involves photosynthetic bio-organic hybrid systems composed of biological components and organic chromophore photosensitizers. Herein, various types of amphiphilic rhodamine B were synthesized to investigate the formation of self-assembly chromophore structures with microscopic and spectroscopic analyses, while hydrogenase expressed ‘Shewanella oneidensis (MR-1)’ bacteria and cationic cellulose nanocrystals (CCNC) as protector of rhodamine B assemblies were added for hydrogen production. We compared aggregation-induced photocatalytic ability dependent on various supramolecular structures of amphiphilic rhodamine Bs, and found out optimal supramolecular chromophore structures and compositions of CCNC and MR-1 for hydrogen production. Through this study, we showed the applicability of chromophore/bacterial complex system for environmentally friendly hydrogen production process.

Poster Presentation : **ENVR.P-705**

Environmental Energy

Event Hall THU 11:00~13:00

Preparation and characterization of chitosan-based porous carbons for carbon dioxide capture

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In this study, porous carbons with high porosity were synthesized by chitosan which known as abundant polysaccharide. The precursors were carbonized at 900℃, 1 hr, and N2 flow conditions using chitosan as carbon precursor. After carbonized, porous carbons were synthesized by chemical activation. The effect on quantity of activation reagents was investigated by experience of carbon precursor/chemical reagent mass ratio. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

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Poster Presentation : **ENVR.P-706**

Environmental Energy

Event Hall THU 11:00~13:00

A study of microporous carbons for high-pressure methane adsorption

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In this study, activated carbons (AC) with high microporosity were synthesized by nitrogen-enriched precursors. The precursors were carbonized at 900℃, 1 hr, and N2 flow conditions. After carbonized, AC was synthesized by chemical activation. The effect of quantity of activation reagents was investigated by experience of AC/chemical reagent mass ratio. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. The microporosities of samples were evaluated using non-local density functional theory (NLDFT). Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

Poster Presentation : **ENVR.P-707**

Environmental Energy

Event Hall THU 11:00~13:00

Facile synthesis of carbon nanotube aerogels for gas adsorption

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Carbon nanotube-based aerogels attract attention due to the high surface area and porosity. In this study, carbon nanotube aerogels were synthesized by carbon nanotubes and chitosan. Chitosan and CNT was dissolved in 1M HCl solution. The Chitosan/CNT mixture were freeze dry for preparing aerogels. Aerogels were carbonized at 200℃, 1 hr, and N2 flow conditions. After carbonized, prepared samples were washed using water and ethanol until neutralization. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. The pore size distributions were investigated using non-local density functional theory (NLDFT).

Poster Presentation : **ENVR.P-708**

Environmental Energy

Event Hall THU 11:00~13:00

Highly sensitive Ammonia (NH3) gas sensor using graphene doped with zinc oxide (ZnO) nanosheet and Tin oxide nano particle, and a method for manufacturing the same

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A highly sensitive Ammonia gas sensor was fabricated using graphene doped with a ZnO Nanosheet and Tin oxide nano particle. The prepared zinc oxide nanosheet and tin oxide nano particle solution doped on graphene. The nano particle solution was prepared by dissolving 10 mg of zinc oxide powder and Tin oxide powder in 2 ml (Etanol) solution. The coating was performed for 300 seconds at a speed of 1000 rpm by dropping 1 to 5 times in a spin-coater. Then, the sample was heated in an oven at 100° C for 30 minutes to remove all volatile organic contaminants. After heating, the prepared Zinc oxide nanosheet and Tin oxide nano particle and graphene composite were cooled for 1 hour, and then mounted on a plastic framework, Connect with silver electrodes. After connecting the electrode of the sensor and the resistance measuring device, Ammonia gas is injected. The Ammonia gas reacts with the sensor in the chamber to change and measure the resistance value of the multimeter equipment. The graphene sensor doped with zinc oxide and Tin oxide nano particle has superior selectivity to Ammonia gas compared to other gases, and has good reproducibility and is sensitive.

Poster Presentation : **ENVR.P-709**
Environmental Energy
Event Hall THU 11:00~13:00

3D Interaction of Zwitterions for Highly Stable and Efficient Inorganic $CsPbI_3$ Solar Cells

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All-inorganic cesium lead iodide ($CsPbI_3$) perovskites, which replace volatile and hygroscopic organic components with stable inorganic cesium cations, have promising photoelectronic properties for potential application in solar cells. However, highly stable, and efficient $CsPbI_3$-based perovskite solar cells are rarely reported because the optically active black phases of $CsPbI_3$ tend to change into a photo-inactive yellow δ-phase. Herein, a highly stable $CsPbI_3$ film that is formed by introducing a small quantity of zwitterions with different dimensions to the perovskite precursor solution is reported. The zwitterions effectively inhibit the formation of the yellow δ-phase during perovskite crystallization and promote the development of a stable black α-phase. In addition, a systematic analysis reveals strong interaction between 3D zwitterions and perovskites in both the solution and film states, which leads to a dense and pinhole-free $CsPbI_3$ film with suppressed trap states. The resulting perovskite solar cells with 3D zwitterions achieve a significantly improved power conversion efficiency of 18.4% with high reproducibility. The devices without encapsulation retain 98% of the initial efficiency after 25 days at 25 °C and relative humidity of 25% ± 5%. Importantly, the 3D zwitterion-based devices demonstrate excellent phase stability when subjected to thermal aging at 100 °C.

Poster Presentation : **ENVR.P-710**

Environmental Energy

Event Hall THU 11:00~13:00

Humidity dependence on deactivation process for photocatalytic VOC_s degradation under UV-illuminated TiO_2

Gahye Shin

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Volatile organic compounds (VOC_s) has affected many air pollution problems, especially, it is toxic for indoor air quality even at small concentrations and is known as a precursor to particulate matter. Therefore, photocatalysis technology has been extensively applied with the development of LED technology for the efficient treatment of (VOC_s). TiO_2 has been investigated as the primary photocatalyst for removing (VOC_s) with economic benefits and sufficient oxidation power. But, the problem of deactivation of the catalysts remains an unsolved problem. The degree of deactivation depends on the structure of (VOC_s). In this work, the chain-type structure of acetaldehyde (C_2H_4O) and ring-type toluene (C_7H_8) were selected to explain the difference as representative materials. Also, the effect of atmospheric humidity on catalytic activity was observed. It is related to the removal efficiency of both substances and has a particular influence on the mineralization of toluene. In this research, we investigated the relationship between the photodegradation behavior of the (VOC_s) and atmospheric humidity based on real-time Fourier transform-infrared (FTIR) analysis. Research of real-time changes with humidity in these (VOC_s) photodegradation reactions can identify the cause of instability of catalysts, which can offer a basis to propel real-life application of photocatalytic technology for removing the harmful (VOC_s) for safe air quality.

Poster Presentation : **ENVR.P-711**
Environmental Energy
Event Hall THU 11:00~13:00

Rapid and portable colorimetric probe for sulfide detection using spiky ball shaped gold nano particles

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Sulfide ion(S^{2-}) pose great harms to not only environment but human due to that can combine with other substances to turn into toxic substances. This situation can easily occur in the vicinity of life and the concentration of sulfides may increase in certain places and conditions that may become more severe. However, the conventional S^{2-} detection method which analytical instrument, fluorescent sensor has several limitation such as working time, moveability, consumption amount and so on. Herein, we presents the possibility of spiky ball shaped gold nano particles(SBNPs) as a rapid and portable colorimetric probe and also protected agent of gold nano particles. SBNPs can be used to colorimetric probe for S^{2-} selectively, and S^{2-} treated SBNPs can endure chemical etching from other toxic anions also. SBNPs colorimetric probe works in 5 minutes at RT. Thereby, we propose SBNPs probe is the way to highly rapid and selective method for detecting S^{2-}, and more simple, easily, high cost efficient and portable than others.

Poster Presentation : **ENVR.P-712**
Environmental Energy
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Photocatalytic CO_2 reduction performances of Eu(III)-doped barium titanate nanoparticles

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Perovskite barium titanate ($BaTiO_3$) has shown a high potential as photocatalysts. Eu(III) ion has been employed as a unique red-luminescence activator in a metal oxide host matrix. Herein, Eu(III)-doped $BaTiO_3$ nanoparticles were synthesized by the hydrothermal method, and their photocatalytic CO_2 reduction activities and products were examined under UVC and UVB light. Major CO_2 reduction products were observed to be CH_3OH, CO, and CH_4 confirmed by gas chromatography. Doped Eu(III) ions were used as a tracer to discuss the roles of dopants by measuring photoluminescence (PL) properties and PL lifetimes. X-ray photoelectron spectroscopy was employed to discuss change in surface chemical states before and after CO_2 reduction tests.

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The dynamic adsorption characteristics of nitrogen containing odorous gases by thermal dried activated carbon after oxidation.

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The study investigates the adsorption kinetics of TDACs (thermal dried activated carbons) based on the NOCs (nitrogen containing odorous gases) adsorption experiments. The NOCs, regarded as the basic odorous gases include ammonia, dimethylamine, trimethylamine, ethylamine, triethylamine, and pyridine. In order to examine the adsorption characteristics, benzene was selected as a non-polar representative for the adsorption test of pristine AC and TDACs. Since the adsorption properties of adsorbents to NOCs and benzene are related to the physicochemical properties of TDAC, the surface properties of the TDACs were characterized by fourier transform infrared (FT-IR) and X-ray photoelectron spectroscopy (XPS). The specific surface area were calculated by N2 /77K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation. The adsorption characteristics were investigated by applying three dynamic adsorption kinetic models (Bohart-adams, Yoon-Nelson and Thomas) to the breakthrough curve of NOCs. The rate constants (K_{BA}) of DMA, EA and TMA on TD 50 were found to as low as 1.68, 1.48 and 1.54 *L/(mg*min)*, respectively, whereas those on pristine AC show the highest value of 24.91, 6.08 and 23.02 *L/(mg*min)*, respectively. Furthermore, a fractal-like kinetic model considering heterogeneous surface characteristics was applied to understand the asymmetric breakthrough curve of NOCs on TDACs. All R square value of breakthrough curve with fractal-like kinetic model were improved. To investigate the gas adsorption selectivity of TDACs, the competitive adsorption was performed by using the TMA in binary mixture.

Poster Presentation : **ENVR.P-714**

Environmental Energy

Event Hall THU 11:00~13:00

Transparent Conducting Oxide Interlayer-free Perovskite/c-Si Tandem Solar Cells

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To solve the issues on environmental pollution and depletion of fossil fuels, research for high-efficiency solar cells has been attracted much attention. A tandem solar cell is being considered as a promising device architecture because it is capable of absorbing light in a wide wavelength range by stacking semiconductor materials having different bandgaps. For developing a tandem structure, it is essential to add an interlayer in which photo-induced electrons and holes recombine at the interface of different semiconductor materials. The interlayer should have excellent electrical conductivity for efficient carrier recombination and high transmittance to allow lots of light to reach the lower light absorption layer, simultaneously. Among various materials, Indium tin oxide (ITO) is commonly used as a conventional interlayer. However, the performance of the ITO layer is restricted due to its parasitic light absorption. Hence, it is necessary to develop a material that can replace ITO for the interlayer. In this study, by controlling the temperature condition of the doping process in forming a P-N junction on the front side of the crystalline silicon, a heavily doped emitter of crystalline silicon solar cell having high electrical conductivity was realized and the emitter layer was applied as the interlayer of the perovskite/c-Si tandem solar cell. As a result, the fabricated perovskite/c-Si tandem solar cell exhibited a power conversion efficiency of over 20% with a high filling factor of 82%, which implies that the heavily doped emitter layer would be a very efficient interlayer of tandem structure.

Poster Presentation : **ENVR.P-715**

Environmental Energy

Event Hall THU 11:00~13:00

Electrochemical CO_2 reduction over transition-metal modified Cd electrodes

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Converting CO_2 into a value-added chemical using an electrocatalyst is a promising strategy that provides long-term energy and environmental solutions. Herein, cadmium (Cd) was used as an electron and tailored by depositing various other transitions metals. CO, H_2, and formate were produced and the relative amounts were controlled by modifying the Cd surface by depositing other transition metals. The Faradaic efficiency (%) was discussed with their physicochemical properties.

Poster Presentation : **ENVR.P-716**

Environmental Energy

Event Hall THU 11:00~13:00

Influence of microporosity on hydrogen storage behaviors of ketjenblack

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In recent years, nanoporous materials with high specific surface areas and porosity have been developed to meet the commercial demands of hydrogen storage systems. In this work, we used Ketjenblack (KB) as a precursor for the production of porous carbon by chemical activation with KOH. KB materials are of great interest because of their lower oxygen content and higher porosity when compared to other porous carbon materials. Activated Ketjenblack (AKB) materials have high specific surface areas (up to 1891 m2 g-1) and various pore sizes (0.46–0.66 nm) in the ultramicropore range. The textural properties of these materials depend strongly on their activation parameters, particularly the KOH/carbon mass ratio. These AKBs achieved hydrogen storage capacities of up to 2.1 wt.% at 1 bar and 77 K, and large heat of adsorption values of up to 8.7 kJ mol-1. The interaction between hydrogen and the carbon surface was more closely related to the porosity than to the surface oxygen content. Among the textural properties of the samples, the pore size and volume were found to be the key factors affecting hydrogen adsorption.

Poster Presentation : **ENVR.P-717**

Environmental Energy

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Mo-doped bismuth vanadate for photoelectrochemical hydrogen production from ammonia decomposition

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Ammonia is considered as a hydrogen carrier because it is easily liquefied at room temperature and has a hydrogen storage capacity of 121 kg/m^3 per unit volume. However, methods to convert hydrogen from ammonia require must be improved to decrease the cost. In the ammonia oxidation reaction, using a photoelectrocatalyst could improve photocatalyst efficiency and produce hydrogen at a low cost. Furthermore, The organic solvent has high solubility in ammonia, so a high concentration of ammonia can be used. The catalytic activity of a typical photoelectric catalyst, the Mo/BiVO$_4$ catalyst was improved in ammonia in this study. It was confirmed that stability and hydrogen generation were increased over the BiVO$_4$ catalyst using Choroamperometry and Gas chromatography.

Poster Presentation : **ENVR.P-718**

Environmental Energy

Event Hall THU 11:00~13:00

Electrocatalytic CO_2 reduction over bismuth film electrodes

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Bismuth (Bi) has shown good electrochemical CO_2 reduction activity and stability. Herein, Bi film electrode was evaluated for electrocatalytic CO_2 reduction at various conditions of different applied potentials, electrolytes, concentration, and UV light. Major product was observed to be formate, and minor products included hydrogen, CO, and CH_4 confirmed by nuclear magnetic resonance spectroscopy and gas chromatography and, respectively. Acetone was also mainly observed at a lower applied potential. Total Faradaic efficiency (%) was observed to be reached closely to 100%. The present study provides valuable information on Bi-based electrodes for electrocatalytic CO_2 reduction of producing value-added carbon products.

Poster Presentation : **ENVR.P-719**

Environmental Energy

Event Hall THU 11:00~13:00

Electrochemical CO_2 reduction over interface-modified Ti-based electrode

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This work presents the electrochemical CO_2 reduction products and Faraday efficiency using transition metal (Cu, Ag, and Au)-modified Ti electrodes. Gaseous products were observed to be H_2, CO, CH_4, and C_2 compounds confirmed by gas chromatography. Their selectivity and Faraday efficiency (%) were evaluated under various experimental conditions of applied potentials, overlayer metal thickness, and electrolytes. This study is expected to provide significant information for the development of electrochemical CO_2 reduction using Ti-based electrodes.

Poster Presentation : **ENVR.P-720**

Environmental Energy

Event Hall THU 11:00~13:00

Ice formation properties of polyol compounds and their applications for hexavalent chromium (Cr(VI)) reduction in ice

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Polyol compounds or sugar alcohols, which are the abundant natural products act as reducing agent against metal ions has been employed as an eco-friendly reductants in the treatment of wastewater. Redox mechanisms of various carbohydrates or sugar alcohols in aqueous solutions have been investigated, however, their effect and reactions in ice have not been reported despite their unique properties to interact with ice nuclei. Polyols interfere with the formation of ice nuclei and hinder the growth of ice crystals on the ice surface. In this study, the interaction of polyol compounds with ice nuclei was investigated, including ethylene glycol, glucose, and trehalose. Also the potential application of the reducing sugar acting as an eco-friendly reducing agent was studied through the removal of the Cr(VI) in Cr(VI)-contaminated wastewater sample in aqueous and ice phases. The results suggest that the purification of the Cr(VI) by polyols through freezing in cold regions.

Poster Presentation : **ENVR.P-721**

Environmental Energy

Event Hall THU 11:00~13:00

Freezing-accelerated hexavalent chromium reduction by ferrous ions and hydrogen sulfide: Kinetics, mechanisms and the environmental relevance

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Freezing, which is the naturally facile phenomenon in the cold climate regions, has been extensively investigated as one of the non-contaminated and cost-effective methods in environmental treatment. The transformation between hexavalent chromium (Cr(VI)), known as more toxic, and trivalent chromium (Cr(III)), known as less toxic, influences hugely on the ecosystems. In this study, we discussed meticulously the process of Cr(VI) to Cr(III) in ice at -20 ºC in comparison with its counterpart in water at 25 ºC through the two reductants available in the environment, which are ferrous (Fe(II)) and hydrogen sulfide (H_2S). Generally, Cr(VI)/Fe(II) and Cr(VI)/H_2S systems happened more rapidly in ice than they did in water. This significant enhancement was attributed predominantly to the freeze concentration effect. The change of Cr(VI) and proton concentrations during freezing was verified using the confocal Raman spectroscopy and UV-Vis spectroscopy with cresol red. The reductive removal of Cr(VI) (20 μM) by Fe(II) and H_2S proceeded appreciably under varying Fe(II) and H_2S concentrations, pH values, and freezing temperatures. These obtained results indicated that the mechanisms of Cr(VI) reduction by Fe(II) and H_2S can make a big contribution to the natural conversion of Cr(VI) in the cold regions. The Fe(II) and H_2S-mediated Cr(VI) reduction in the frozen Cr(VI)-contaminated wastewater showed the same trend as those in the frozen Cr(VI) solution. This finding implies that the existence of substrates affected merely the Cr(VI) conversion rate in ice. Therefore, Cr(VI)/Fe(II)/freezing and Cr(VI)/H_2S/freezing systems can be applied promisingly for Cr(VI)-contaminated wastewater treatment.

Poster Presentation : **ENVR.P-722**
Environmental Energy
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Oxygen-tolerant nitrate conversion using TiO_2 composite modified with bimetals and Cr_2O_3

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The quantitative conversion of nitrate (NO_3^-) to dinitrogen (N_2) in oxygen dominant environment seems to be almost impossible and regarded as a limitation for the practical application of photocatalysts. Herein, the special-purpose ternary composite (Cr_2O_3/Ag-Pd/TiO_2) was synthesized and firstly evaluated as a superior photocatalyst for highly selective nitrate reduction under the ambient aerated condition without using any chemical reductants. The oxygen-tolerant nitrate conversion proceeded through overall water splitting by utilizing in situ generated H_2 as a sole reductant and NO_3^- can be subsequently transformed to N_2. The introduction of Cr_2O_3 shell perfectly inhibited accumulation of bulky O_2 molecules around the catalyst and accelerated protons and electrons coupled transfers. The reduction of NO_3^- and NO_2^- was possible because of electrons provided from silver nano particles, which reduces Ti^{5+} to Ti^{4+} and protons to H_2 under the light irradiation and is an underlying reason for the increased N_2 yield. Ag particles are significantly involved in O_2 generation in Cr_2O_3/Ag-Pd/TiO_2 composite by their redox-mediated shuttles. Cr_2O_3/Ag-Pd/TiO_2 was able to remove 100% of NO_3^- during the 12 h photoreaction with 90% selectivity to N_2 under ambient aerated water. Our findings provide a suitable platform for investigating how to scale up the solar denitrification in the presence of dissolved oxygen.