Plenary Lecture : **PLEN-1**
Plenary Lecture
Room 301 (Live Streaming) MON 11:00

DNA-mediated Signaling through Redox Chemistry

Jacqueline K. Barton

John G. Kirkwood and Arthur A. Noyes Professor of Chemistry , California Institute of Technology, United States

Many experiments have now shown that double helical DNA may serve as a conduit for efficient redox chemistry over long molecular distances. This chemistry is exquisitely sensitive to perturbations in the DNA base stack, such as arise with base mismatches, lesions, and protein binding. We have explored how this chemistry may be used within the cell for long range signaling. Increasingly, 4Fe-4S clusters are being found in DNA-binding proteins involved in genome maintenance. These 4Fe-4S clusters, common redox cofactors, are associated not only with repair proteins but also DNA polymerases and primase. Studies are described to characterize DNA–mediated charge transport by these metalloproteins. Experiments indicate that this chemistry is important in the context of oxidative damage and also may provide a first step in how DNA repair proteins may localize in the vicinity of lesions. This redox chemistry at a distance, mediated by the DNA helix, offers a route for long range signaling among DNA-processing proteins across the genome.

Award Lecture : **AWARD-1**

2020 Taikyue Ree Academic Award

Room 301 (Live Streaming) WED 11:30

Chair: Jeung Gon Kim (Jeonbuk National University)

New Methodologies for Construction of Biologically Interesting Aromatics and Heteroaromatics

Yong Rok Lee

Division of Chemical Engineering, Yeungnam University, Korea

The construction of various functionalized aromatic and heteroaromatics via annulation and C-H activation plays a vital role in advanced synthetic organic chemistry. These compounds have shown a lot of biological activities and widely used for the development of new drugs and functional materials. Owing to their importance and usefulness, we have been interested in the synthesis of aromatics and heteroaromatics utilizing new methodologies. In this presentation, we describe a facile and efficient construction of biologically interesting and diverse aromatics and heteroaromatics via annulation and C-H activation developed by our group (Scheme 1).1-10

Reference

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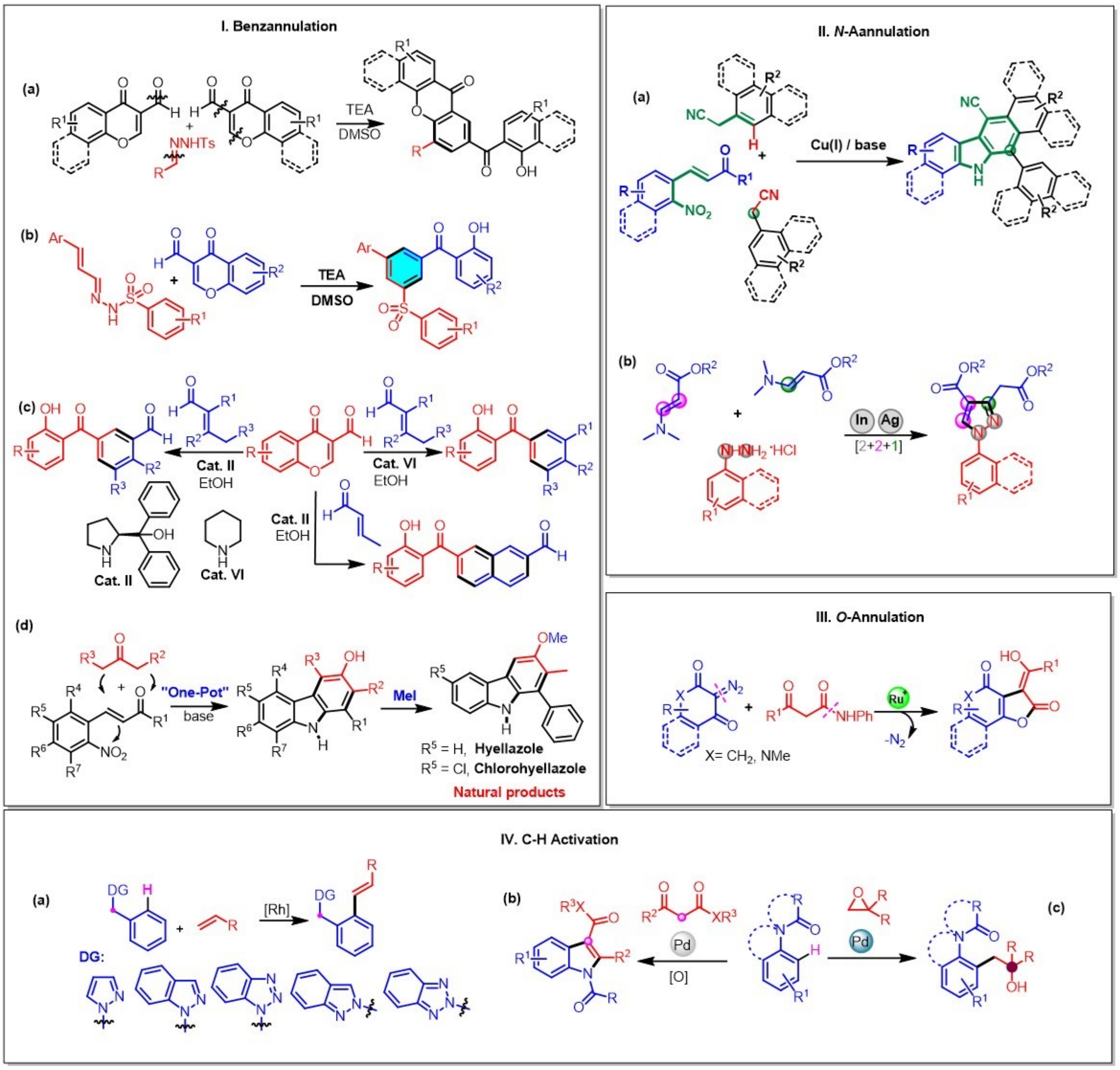
10.Thombal, R. S.; Feoktistova, T.; González-Montiel, G. A.; Cheong, P. H.-Y.; Lee, Y. R. Chem. Sci. 2020, 11, 7260.



Scheme 1. Synthetic strategies for aromatics and heteroaromatics

Symposium : **KCS1-1**
[International Symposium] The Future is Already Here: Advancing Frontiers in Chemical Research
Room 301 (Live Streaming) MON 13:30
Chair: Eunsung Lee (POSTECH)

Sound, Chemistry, and Patterns

Kimoon Kim

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

Naturally occurring spatiotemporal patterns typically have a predictable pattern design and are reproducible over several cycles. However, the patterns obtained from artificially designed out-of-equilibrium chemical oscillating networks (e.g. Belousov-Zhabotinsky (BZ) reaction), are unpredictable and difficult to control spatiotemporally, albeit reproducible over subsequent cycles. Recently, we showed that it is possible to generate reproducible spatiotemporal patterns in out-of-equilibrium chemical reactions and self-assembling systems in water in the presence of sound waves, which act as a guiding physical stimulus. Audible sound-induced liquid vibrations control the dissolution of atmospheric gases (e.g. O_2, CO_2) in water to generate spatiotemporal chemical patterns in the bulk of the fluid, segregating the solution into spatiotemporal domains having different redox properties or pH values. It further helps us in the organization of transiently formed supramolecular aggregates in a predictable spatiotemporal manner. Details of this work will be presented.

Symposium : **KCS1-2**

[International Symposium] The Future is Already Here: Advancing Frontiers in Chemical Research

Room 301 (Live Streaming) MON 14:10

Chair: Eunsung Lee (POSTECH)

Mechanism-Driven C-H Amidation: Reaction Development and Asymmetric Catalysis

Sukbok Chang

Department of Chemistry, Institue for Basic Scicence and 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 : **KCS1-3**
[International Symposium] The Future is Already Here: Advancing Frontiers in Chemical Research
Room 301 (Live Streaming) MON 15:00
Chair: Eunsung Lee (POSTECH)

HÜCKEL, MÖBIUS, BAIRD AND 3-DIMENSIONAL AROMATICITY IN VARIOUS EXPANDED PORPHYRINS

Dongho Kim

Department of Chemistry, Yonsei University, Korea

Modification of aromaticity is regarded as one of the most interesting and important research topics in the field of physical organic chemistry. Particularly, porphyrins and their analogs (porphyrinoids) are attractive molecules for exploring various types of aromaticity as most porphyrinoids exhibit circular conjugation pathways in their macrocyclic rings with various molecular structures. Aromaticity in porphyrinoids is significantly affected by structural modification, redox chemistry, NH tautomerization, and electronic states (singlet and triplet excited states). Conversely, aromaticity significantly affects the spectroscopic properties and chemical reactivities of porphyrinoids. Up to date, considerable efforts have been devoted to understanding and controlling the aromaticity and antiaromaticity of porphyrinoids. Thus, a series of porphyrinoids are in the limelight being expected to shed light on this field because they have some advantages to demonstrate the switching of aromaticity; it is possible to control the aromaticity by lowering the temperature, adding and removing the protons of expanded porphyrins, changing the chemical environment, and switching the electronic states (triplet and singlet excited states) by photoexcitation. In this regard, this presentation will address the control of aromaticity in various expanded porphyrins from the spectroscopic point of view with assistance from theoretical calculations.

Symposium : **KCS1-4**
[International Symposium] The Future is Already Here: Advancing Frontiers in Chemical Research
Room 301 (Live Streaming) MON 15:40
Chair: Eunsung Lee (POSTECH)

Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry

Wonwoo Nam

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

Dioxygen is essential in life processes, and enzymes activate dioxygen to carry out a variety of biological reactions. One primary goal in biomimetic research is to elucidate structures of reactive intermediates and mechanistic details of dioxygen activation and oxygenation reactions occurring at the active sites of enzymes, by utilizing synthetic metal-oxygen complexes. A growing class of metal-oxygen complexes, such as metal–superoxo, –peroxo, –hydroperoxo, and –oxo species, have been isolated, characterized spectroscopically, and investigated in various oxygenation reactions. During the past decade, we have been studying the chemical and physical properties of various reactive intermediates in oxygenation reactions, such as high-valent iron(IV)- and manganes(V)-oxo complexes of heme and non-heme ligands in oxo-transfer and C-H activation reactions, non-heme metal-peroxo complexes in nucleophilic reactions, and non-heme metal-superoxo complexes in electrophilic reactions. The effects of supporting and axial ligands on structural and spectroscopic properties and reactivities of metal-oxygen adducts have been extensively investigated as well. In this presentation, I will present our recent results on the synthesis and structural and spectroscopic characterization of mononuclear nonheme metal-dioxygen intermediates as well as their reactivities in electrophilic and nucleophilic oxidation reactions.

Symposium : **KCS1-5**

[International Symposium] The Future is Already Here: Advancing Frontiers in Chemical Research

Room 301 (Live Streaming) MON 16:20

Chair: Eunsung Lee (POSTECH)

Nanomaterials Toolkit for Next Generation Imaging and Cell Manipulations

Jinwoo Cheon

Center for Nanomedicine, Institute for Basic Science (IBS), Korea

Nanoscience has become a critical component for the innovtions in biomedical sciences and the new development in nanoscale concepts and tools that can accurately image, identify, and execute desired missions of biological systems are of importance. In this talk, I will discuss nanomaterials as core platform tools for a variety of functionalities such as sensing, targeting and signaling control of cells in selective and unprecendelty efficient ways. Their unique utilizations in highly accurate bio-imaging, point-of-care genetic sensing for viral detection, and molecular level cell signaling and fate control will be discussed in detail.

Symposium : **KCS4-1**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 13:30
Chair: Kangkyun Baek (Institute for Basic Science)

New Paradigm for Cell Identification

Young-Tae Chang

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

Our body is composed of many, and many different kinds of cells. The distinction of different cells is the starting point of understanding the role of each cell in the higher complexity of cell community, i.e. an organism. The current cell labeler is based on small molecule-target recognition, so called Paul Ehrlich's magic bullet model. We may call this kind of probe as Holding Oriented Live-cell Distinction (HOLD) probe.Another possibility is Maxwell's demon model. If the reporter molecule is selectively uptaken by a specific gating protein to a cell, we may call this kind of probe as Gating Oriented Live-cell Distinction (GOLD) probe. Specific example with activated macrophage probe, CDg16 will be presented for GOLD and the probe will be available to the community for free.

Symposium : **KCS4-2**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 13:55
Chair: Kangkyun Baek (Institute for Basic Science)

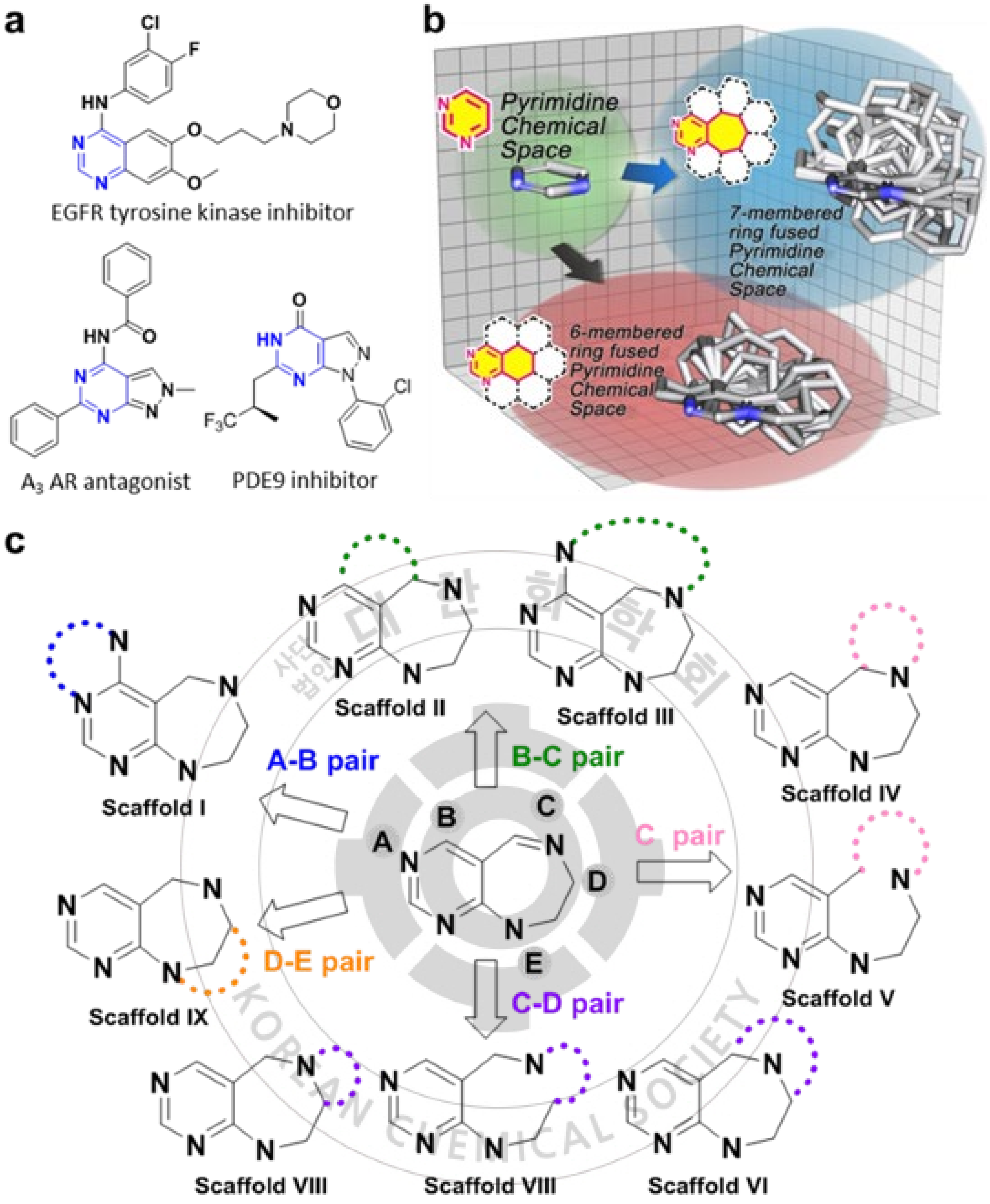
Design and Synthesis of Novel Molecular Diversity for the Study of Protein-Protein Interactions

Seung Bum Park

Division of Chemistry, Seoul National University, Korea

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. However, the design and synthesis of small-molecule libraries with improved biological relevance as well as maximized molecular diversity represents a key challenge. Herein, we employ functional group pairing strategy for the diversity-oriented synthesis of a chemical library containing privileged substructures, pyrimidodiazepine or pyrimidine moieties, as chemical navigators toward unexplored bioactive chemical space. This presentation highlights that privileged substructure-based DOS (pDOS) strategy can be a powerful research tool for the construction of drug-like compounds to address challenging biological targets.

References:[1] Kim, J.; Kim, H.; Park, S.B.* J. Am. Chem. Soc. 2014, 136(42), 14629–14638 [2] Choi, Y.†; Kim, H.†; Shin, Y.-H.; Park, S.B.* Chem. Comm. 2015, 51, 13040–13043[3] Kim, C.†; Jung, J.†; Tung, T.T.; Park, S.B.* Chem. Sci. 2016 7, 2753–2761.[4] Kim, J.; Koo, J.; Jung, J.; Cho, W.; Kim, C.; Park, W.; Park, S.B.* Nat. Comm., 2016; 7: 13196.[5] Koo, J.; Kim, J.; Park, S. B.* Org. Lett., 2017, 19, 344–347.[6] Choi, Y.†; Kim, H.†; Park, S. B.* Chem. Sci., 2019, 10, 569–575* Fill in this blank within 1800 byte (In case of including Figures: within 1400 byte)* Attached Figures below (next page)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Pyrimidine Chemical Space
7-membered ring fused Pyrimidine Chemical Space
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B-C pair
C pair
C-D pair
D-E pair
A
B
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Symposium : **KCS4-3**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 14:20
Chair: Kangkyun Baek (Institute for Basic Science)

A protocell as a molecular network system mimicking intracellular protein aggregation and its intra- and intercellular effects

Kyeng Min Park

Center for Self-assembly and Complexity, Institute for Basic Science, Korea

Undesirable aggregation of intrinsically disordered proteins including tau protein and α-synuclein causes progressive death of neuronal cells as neurodegenerative diseases including Alzheimer's and Parkinson's disease. The protein aggregation in cells and tissues is known to be promoted by oxidative stress under acidic conditions and affects the integrity of organellular and cellular membranes. However, the complex nature of physiological environments has hampered the deep investigation of the effect of the protein aggregation to the membranes causing propagative cell death. Recently, cell-like artificial microcompartments have been intensively investigated as protocells (or artificial cells) for better interrogating and understanding of cellular functions and behaviors of interest in a simplified form. A rational organization of chemical and biological components in a compartment allowed the construction of protocells mimicking important cellular functions and behaviors under a well-defined and controllable condition. Until recently, little effort has been devoted to construct a protocell that mimics destabilization of biological membranes by protein aggregation despite its heavy involvement in neurodegenerative diseases. In this talk, I will present our recent efforts to provide a giant unilamellar vesicle as a protocell mimicking destabilization of biological membranes by intracellular protein aggregation in a controllable manner. In addition, the intra- and intercellular effects of the protein aggregation to organelle and other cell mimics in a simplified system will be discussed.

Symposium : **KCS4-4**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 14:35
Chair: Kangkyun Baek (Institute for Basic Science)

Current issues in molecular dynamics simulations of biomolecular self-assembly

Jejoong Yoo

Department of Physics, Sungkyunkwan University, Korea

In biology and chemistry, self-assembly is a fundamentally important process that enables the formation of macromolecules and supramolecules, respectively. Because inter-atomic interactions determine the self-assembly processes, atomic differences in the unit molecules can lead to a dramatically different self-assembly process. A good example is the two fundamental classes in biology—nucleic acids and amino acids—that differ from each other within a class by only a few atoms. Thus, the molecular dynamics (MD) simulation that can distinguish each atom became a mainstream computational tool in self-assembly. In this talk, we will evaluate the current issues in the MD simulation of self-assembly based on the principles of physical chemistry. Specifically, we will show that the colligative properties of small model compounds such as osmotic pressure can serve as an ideal reference data to evaluate and enhance the accuracy of the intermolecular interactions quantitatively. Then, we will demonstrate that the newly optimized force field can dramatically improve the realism of the MD simulations of various biological systems, including protein folding, DNA condensation, and protein-DNA complexes.

Symposium : **KCS4-5**

[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly

Room 301 (Live Streaming) WED 15:05

Chair: Minyoung Yoon (Kyungpook National Univeristy)

Forming Two- and Three-Dimensional Organic Network Structures for Various Applications

Jong-Beom Baek

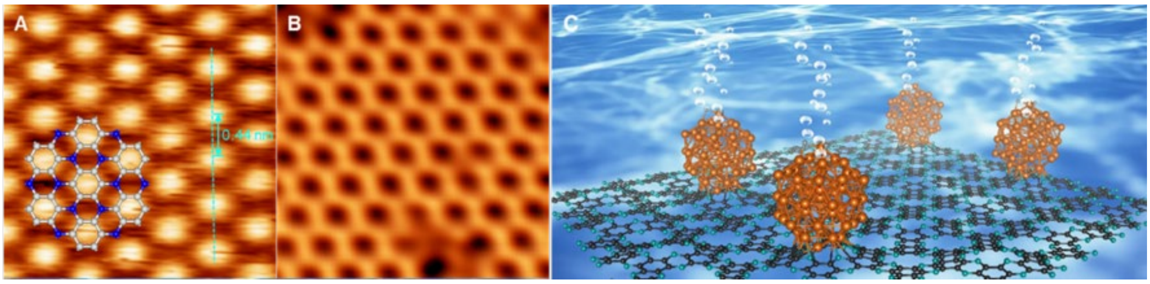
Division of Energy Engineering, Ulsan National Institute of Science and Technology, Korea

Robust conjugated two- (2D) and three-dimensional (3D) non-metallic network polymers have attracted immense interest due to their unusual electronic, optoelectronic, magnetic and electrocatalytic properties. In addition, their tunable structures and properties promise to offer many opportunities in various applications. However, even after years of intensive exploration in science and technology, facile and scalable methods capable of producing fused-aromatic based stable non-metallic network polymers with uniformly decorated heteroatoms with/without holes remain limited. To overcome these issues, stable organic network polymers have been designed and synthesized. They have uniformly distributed heteroatoms,1 holes with heteroatoms2 and transition metal nanoparticles in the holes.3 Their network structures were confirmed using various characterization techniques, including scanning tunneling microscopy (STM, Figure 1). Based on the stoichiometry of 2D layered network polymers, they were, respectively, designated C2N, C3N, C4N, and M@C2N (M = Co, Ni, Pd, Pt, Ru). Their electronic and electrical properties were evaluated by electrooptical and electrochemical measurements along with density-functional theory (DFT) calculations. Furthermore, robust 3D cage-like organic network polymers have also been constructed and they show high sorption properties.4,5 The results suggest that these newly-developed 2D and 3D organic network polymers offer greater opportunities, from wet-chemistry to various device applications.

References:[1] Mahmood, et al. Two-dimensional polyaniline (C3N) from carbonized organic single crystals. Proceedings of National Academy of Sciences, USA 2016, 113, 7414.[2] Mahmood, et al. Nitrogenated holey two-dimensional structure. Nature Communications 2015, 6, 6486.[3] Mahmood, et al. An efficient and pH-universal ruthenium-based catalyst for the hydrogen evolution reaction. Nature Nanotechnology 2017, 12, 441.[4] Bae, et al. Forming a three-dimensional porous organic network via explosion of organic single crystals in solid-state. Nature Communications 2017, 8, 159-Highlighted in

Nature Nanotechnology 2018, 13, 4.[5] Mahmood, et al. A robust 3D cage-like ultramicroporous network structure with high gas uptake capacities. Angewandte Chemie International Edition 2018, 57, 3415.

Figure 1. STM images: A, C3N; B, C2N. C, Schematic representation of Ru@C2N.



Symposium : **KCS4-6**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 15:30
Chair: Minyoung Yoon (Kyungpook National Univeristy)

Covalent Self-assembly of Unconventional Nano/microstructures

Kangkyun Baek

Center for Self-assembly and Complexity, Institute for Basic Science, Korea

Despite the potential to generate robust and stable architectures, the use of strong covalent bonds was typically disfavored in the synthesis of the well-defined nano- and micro-architectures mainly due to slow kinetics or lack of self-error-correction process. Over the last decade, continuous effort has been devoted to the investigation of molecular design principle and reaction conditions, which allows us to successfully demonstrate the self-assembly of unconventional nano/microarchitectures, such as molecular polyhedrons, nanocapsules, single-layer films, and hollow nanotubular toroidal microrings, via covalent bond formation. Recently, we have also construct graphene-like π-conjugated polymer films with long range internal order and high charge carrier mobility via in-situ autoxidation and subsequent reversible condensation reactions involving a final irreversible ring-closure reaction. More details of the work will be presented.

Symposium : **KCS4-7**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 15:45
Chair: Minyoung Yoon (Kyungpook National Univeristy)

Sound-controlled Spatiotemporal Patterns in Out-of-equilibrium Systems

Ilha Hwang

Center for Self-assembly and Complexity, Institute for Basic Science, Korea

Patterns emerge everywhere and scientists have been studying them to better understand nature. Among such studies, chemists are particularly interested in spatiotemporal patterns that are formed and changed by chemical reactions. However, in ensembles of synthetic chemical systems, the patterns resulting from the diffusion of chemicals are not predictably controlled so far. To address this issue, we used audible sound as a guiding stimulus to control the dissolution, diffusion and transport of chemicals in out-of-equilibrium chemical reaction system and obtained predictable spatiotemporal patterns. Our strategy segregates a solution into spatiotemporal domains, differing in their redox or pH properties without the use of any compartmentalization-aiding motif. In addition to the colored patterns, it further helps us in organizing supramolecular aggregates along these redox- or pH-specific domains in a solution. In this talk, I will present recent findings on the sound-controlled pattern formation and their applications.

Symposium : **KCS4-8**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 16:00
Chair: Minyoung Yoon (Kyungpook National Univeristy)

Chemical Fuel-Driven Transient Crystallization

Rahul Dev Mukhopadhyay

Center for Self-assembly and Complexity (CSC), Institute for Basic Science, Korea

Fuel-driven self-assembling systems are ubiquitous in nature. Among these, a widely cited example is the formation-deformation mechanism of microtubules via the self-assembly of tubulin proteins fueled by guanosine-5’-triphosphate (GTP). In case of artificially designed fuel-driven, transient self-assembling systems, they often suffer from the accumulation of chemical wastes that interfere with the formation of pristine self-assembled products in subsequent refueled cycles. Recently we discovered that the chemical fuel-driven transient crystallization of a cucurbit[8]uril-based host-guest complex, can be efficiently carried out avoiding the large accumulation of chemical wastes in solution. Here we made use of trichloroacetic acid as a fuel, which undergoes base-catalyzed thermal decarboxylation producing volatile chemical wastes that are spontaneously removed from the solution.1 As a result of such a self-clearance process, the minimal presence of chemical wastes does not significantly influence the formation, morphology and structural integrity of the crystals. Details of our research in this area will be presented.

References1. Choi, S.; Mukhopadhyay, R. D.; Kim, Y.; Hwang, I. -C.; Hwang, W.; Ghosh, S. K.; Baek, K.; Kim, K. Angew. Chem. Int. Ed. 2019, 58, 16850-16853.

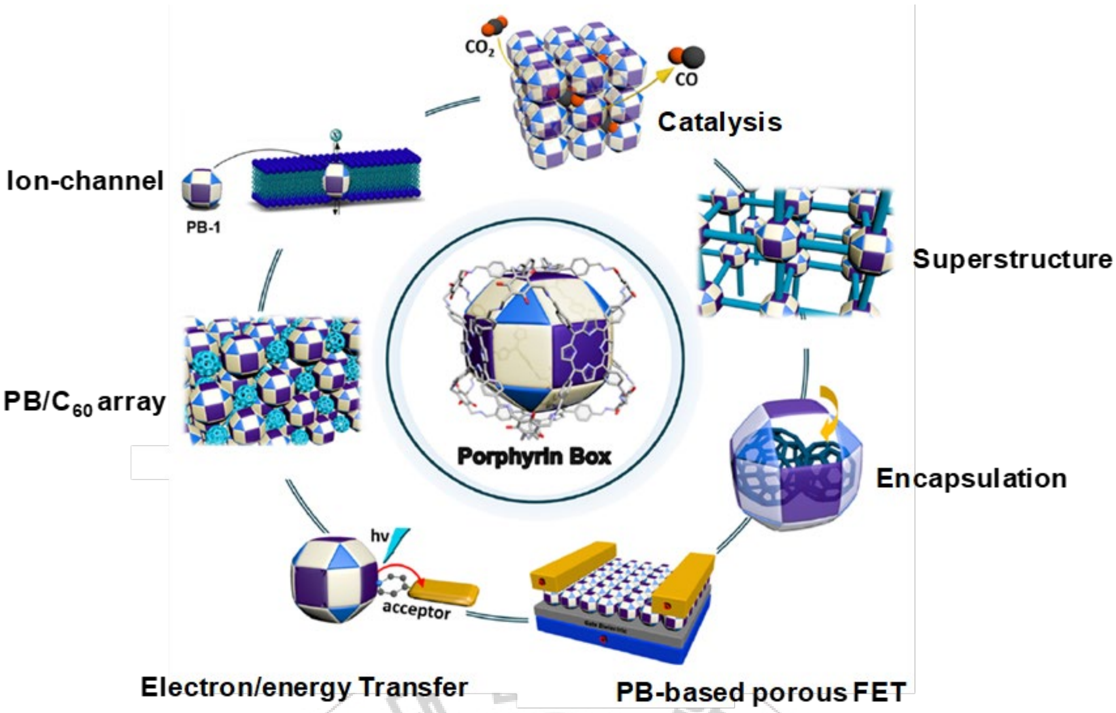
Symposium : **KCS4-9**
[IBS Symposium] Frontiers in Molecular Recognition and Self-assembly
Room 301 (Live Streaming) WED 16:15
Chair: Minyoung Yoon (Kyungpook National Univeristy)

Porphyrin Boxes and Beyond

Younghoon Kim

Center for Self-assembly and Complexity, Institute for Basic Science, Korea

In 2015, we reported the rationally designed organic cages, named as porphyrin boxes (PBs), using six square shaped porphyrin units and eight triangular building blocks. PBs are cube-shaped, shape-persistent porous organic solids with a large cavity (~2 nm in diameter). The size of pore can be tuned using different sized building units while maintaining the topology of the cages. Beside the high chemical stability in a broad pH range (4.8 to 13) in aqueous media, the PBs exhibit a high surface area (1370 m2g-1) and interesting gas sorption behavior in the solid state. By virtue of the unique properties, we have been exploring many fields such as selective ion transport, catalysis, and the construction of hierarchical superstructures. Recent results on porphyrin boxes and other related self-assembled organic cages will be presented.


CO$_2$
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PB-1
Superstructure
Porphyrin Box
PB/C$_{60}$ array
Encapsulation
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Electron/energy Transfer
PB-based porous FET

Symposium : **KCS5-1**
[KCS-SK innovation Joint Symposium] Green Chemistry for Social Value
Room 306 (Live Streaming) WED 13:00
Chair: Jongho Lim (SK Innovation)

The development of new strong Brønsted acids and their applications

Lee Sunggi

Department of Emerging Material Science, Daegu Gyeongbuk Institute of Science & Technology, Korea

The development of environment-friendly and sustainable catalysts has attracted a great attention from academia and industry. Since late 1990s, organocatalysts were exploited due to its non-toxic character. The phosphoric acids and secondary amine catalysts initiated and more and more organic molecule-based catalysts were developed. Compared to transition-metal catalysts, the organocatalyst system was suffered by its low efficiency and limited applications utilizing highly reactive intermediates. In this presentation, I will share the development of new strong Brønsted acids, imidodiphosphoramides (IDPi) and their applications, which overcome long-standing limitations. The new organocatalysts enabled various challenging reactions which cannot be achieved with conventional organo- and transition-metal catalysts especially in enantioselective reactions.

Symposium : **KCS5-3**
[KCS-SK innovation Joint Symposium] Green Chemistry for Social Value
Room 306 (Live Streaming) WED 15:00
Chair: Jongho Lim (SK Innovation)

Photoelectrochemical CO2 Reduction into Liquid Fuels: Thermodynamics and Kinetics Control

Young soo Kang

Department of Chemistry, Sogang University, Korea

Photoelectrochemical (PEC) system for the reduction of CO2 into liquid fuels of formaldehyde and acetaldehyde with minor hydrogen gas bubbling has been described in the aspect of thermodynamics and kinetics of the CO2 reduction reaction to have efficient method by lowering activation energy of CO2 reduction on the electron transfer reaction and to do reduction potential tuning of CO2 reduction reaction for the selective reduction products. Ca/Fe doped TiO2 photoanode oxidizes water and generates the large amount of O2, electrons and protons. On the other side, rGO(reduced graphene oxide)/PVP(poly(4-vinyl)pyridine)/Nafion multi-layers have been coated and fabricated on the surface of Cu foil cathode to reduce CO2 into formaldehyde and acetaldehyde. When solar light was irradiated on the surface of photoanode, electrons get excited to the conduction band of Ca/Fe doped TiO2 and transported to the cathode via external wire with low external bias potential. rGO on Cu foil has been used for the dual functions of reduction potential tuning and multi-electron shuttling process of CO2 reduction reaction. The multi-electron shuttling function was illuminated by larger number and longer life-time of excited electrons and generating electron cloud, which have been confirmed by time-resolved photoluminescence (TR-PL) decay curves and 2D time-resolved photoluminescence (TR-PL) mapping images of Cu/rGO electrode. This allows the sequential multi-electron transport process from Cu/rGOcathode to CO2, which was studied with time-resolved chronoamperometry. N-heterocyclic poly(4-vinyl)pyridine (PVP) helps to capture and do chemical activation of reactant CO2 molecule by complexation as [PVP-CO2*] complex via charge separation and lowering transition state energy level of the electron transfer for the formation of anion radical of carbon dioxide complex with PVP as [e- + PVP-CO2*]≠ complex via electron delocalization, which is basically possible due to high basicity of lone pair electrons of nitrogen atoms of N-heterocyclic PVP compounds. These functions result in the lowered activation energy for the CO2 reduction reaction to have faster kinetics. The decreased amount of activation energy was determined with Tafel plots by measuring the slopes of it and semicircles of the electrochemical impedance spectroscopy (EIS) Nyquist plots at different temperatures. Nafion film coated on the surface of cathode assists the faster transport of H+ ions to CO2 reduction reaction sites for the simultaneous one-pot reaction of proton coupled electron transfer reactions.

Award Lecture in Division : **POLY1-1**

Special Symposium by Mid-career Polymer Synthesis Scientists

Room 402 (Live Streaming) TUE 10:40

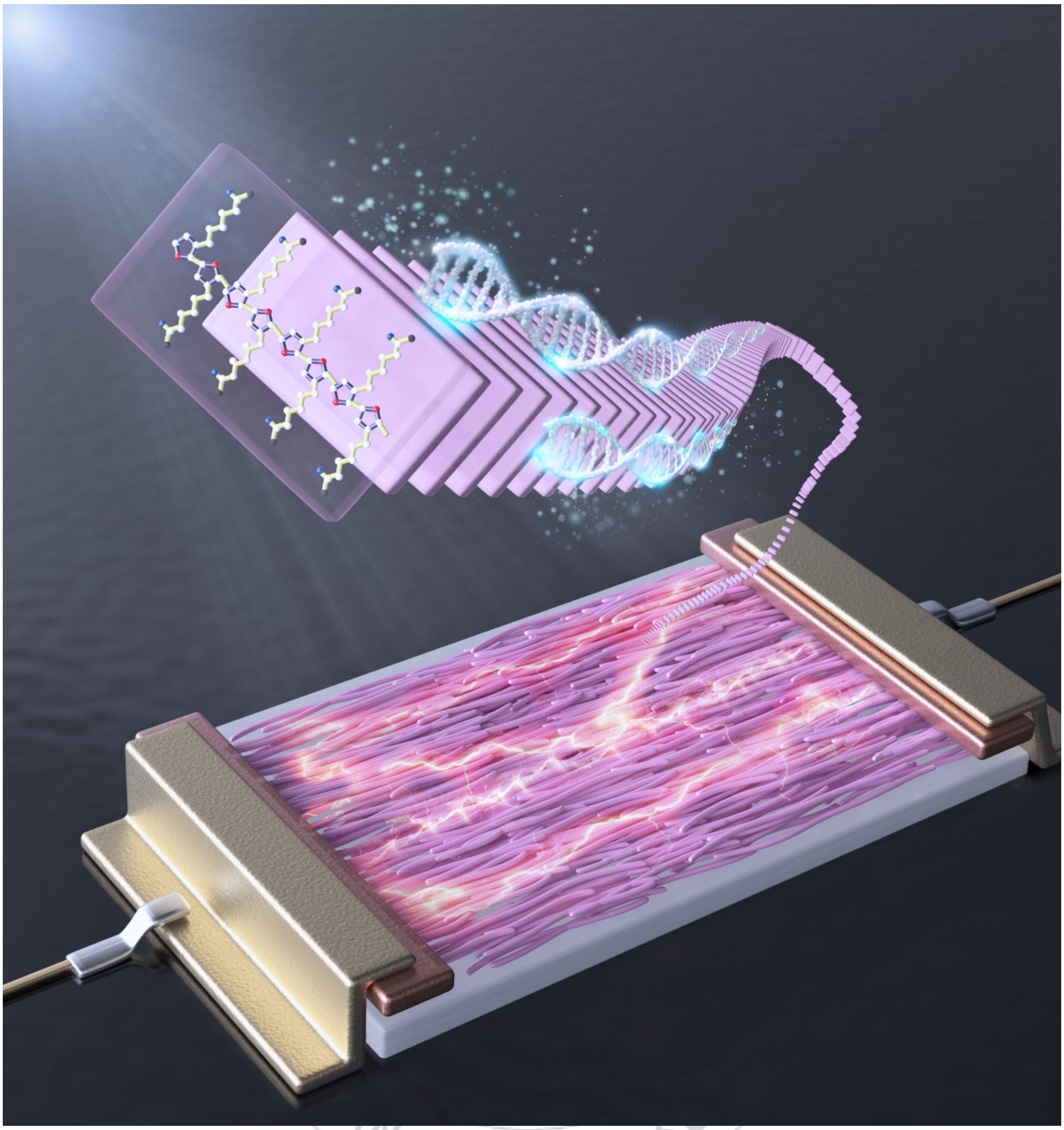
Chair: BongSoo Kim (UNIST)

Orientation control of polymeric materials for optical and electronic applications

Dong Ki Yoon

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

The orientation control of biomaterials and organic semiconductors is of fundamental importance to anisotropic optical and electronic behavior as well as high performance in the practical applications. Here, we demonstrate high-performance organic field-effect transistors (OFETs) based on semiconducting polymers with orientation control from molecular- to micro-scale dimensions, using self-organized DNA templates and line-patterned PDMS molds, respectively. In the systems, the charge carrier mobility of polythiophene derivatives is correlated with their orientation, which related to inter- and intramolecular charge transport: the mobility of them along the π-conjugation direction is ~ 2 orders of magnitude higher compared to the randomly oriented condition. The platforms provide important insight and guidelines for the design of organic optoelectronic devices with high performance and tunability.



Symposium : **POLY1-2**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 402 (Live Streaming) TUE 11:10
Chair: Minjae Lee (Kunsan National University)

Development of Flexible Hard Coating with Anti-fingerprint (AF) Surface

Bongjin Moon

Department of Chemistry, Sogang University, Korea

As the new era of the flexible display comes, new materials with totally unmet specifications are required. One of the examples is a flexible hard coating that can replace the role of traditional cover glass windows in display devices. Theoretically, it is very challenging to develop a material that can exhibit glass-like hardness and rubber-like flexibility at the same time. To realize such properties, we have attempted various strategies integrating both nano-scaled hard segments and soft segments. Choosing an appropriate combination of the materials for both hard- and soft-segments was critical to obtain the desired hardness and softness of the final coating. Besides, we have designed and synthesized new per-fluorinated additives that can form an anti-fingerprint (AF) surface on the hard coating film by the simple solvent-annealing process.

Symposium : **POLY1-3**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 402 (Live Streaming) TUE 11:35
Chair: Minjae Lee (Kunsan National University)

Synthesis and Applications of Stimulus-responsive Conjugated Polydiacetylenes

Jong-Man Kim

Department of Chemical Engineering, Hanyang University, Korea

The interest in chromogenic conjugated polymers that change their visual appearance in response to external stimulus has gained special attention for the devising and developing sensor systems. Polydiacetylenes (PDAs), obtained by topochemical polymerization of self-assembled diacetylene (DA) monomers, encompass extended π-conjugated functionality and absorb light typically in the visible region with a brilliant blue color appearance. Since no catalysts or initiators are required for the topochemical polymerization; PDAs are formed with a high degree of purity which makes them suitable for direct implementation and designing devices in different shapes including coatings, films/sheets, fibers/wires and vesicles. The unique property of nanostructured PDA that leads to their application as sensing elements is the occurrence of a color (typically blue-to-red) and fluorescence (non-to-red) changes that take place in response to a variety of environmental perturbations such as heat, solvent, mechanical stress, pH, and specific ligand-receptor interactions. In this symposium, recent advances in the area of nanostructured PDA-based chemosensors focused on our results will be presented.

Symposium : **POLY1-4**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 402 (Live Streaming) TUE 12:00
Chair: Minjae Lee (Kunsan National University)

Artificial Opal Platform Technology for Photonic Gel Sensors

Wonmok Lee

Department of Chemistry, Sejong University, Korea

There have been recent reports on photonic gel sensors, fabricated using an artificial opal templating method, that rely on reversible changes in the reflective color in response to the binding of the analyte to the receptor tagged to the hydrogel. Two essential features of a photonic gel sensor are (1) the existence of external stimuli (either chemical or field) to induce a solvent influx and subsequent volume changes of the hydrogel, and (2) periodic variations of refractive indices within the opal-templated hydrogel at the submicron length scale exhibiting various reflective colors with specific stimuli. Since the reflective color originates from the periodic structure of the hydrogel, it is often called the structural color. In this presentation, we present an artificial opal platform technology for the fabrication of inverse opal photonic gel sensors exhibiting fast responses to various stimuli. Recent developments of photonic gel sensors from two different fabrication approaches of photonic film and photonic ball will be discussed.

Symposium : **POLY1-5**
Special Symposium by Mid-career Polymer Synthesis Scientists
Room 402 (Live Streaming) TUE 12:20
Chair: Minjae Lee (Kunsan National University)

Tuning the thermoelectric properties of two dimensional materials using an electrochemical transistor

Hyunjung Lee

School of Advanced Materials Engineering, Kookmin University, Korea

Reduced graphene oxide (rGO) possesses a similar electronic structure to graphene but can be synthesized on a larger scale. Hence, rGO is considered as an attractive alternative to graphene. Here we report the carrier transport properties of thermally reduced graphene oxide (TrGO) as a function of reduction temperature. The transfer curve of a field effect transistor fabricated with TrGO exhibited ambipolar properties, and the charge neutrality point of TrGO was shifted from negative to positive as the reduction temperature increased. Furthermore, as revealed in Arrhenius plots of the carrier densities and carrier mobilities, TrGO behaved as a metallic conductor at all reduction temperatures. To investigate the effect of reduction temperature on the thermoelectric properties of TrGO, the Seebeck coefficients of the fabricated TrGOs were calculated from the transfer curve using Mott's equation for metallic materials. At a sufficiently high reduction temperature, the Seebeck coefficient switched sign from negative to positive, indicating that electron and hole carrier transport dominates at higher and lower reduction temperature, respectively. The calculated Seebeck coefficients at zero gate bias were compared with the measured coefficients in TrGO bulk films. The thermoelectric properties of the measured and calculated coefficients showed similar trends with increasing reduction temperature, and the charged carrier transport (i.e., the energy states) of TrGO can be tuned by varying the reduction temperature without doping with impurities.

Symposium : **POLY2-1**
Recent Trends in Early-career Polymer Chemists
Room 402 (Live Streaming) TUE 13:30
Chair: Min Sang Kwon (Seoul National University)

Gel-state Electrolytes for Lithium Batteries

Jin Hong Lee

School of Chemical Engineering, Pusan National University, Korea

With the ever increasing demand for next generation electrochemical energy storage cells to achieve higher performance, often overlooked are the safety issues arising from electrolytes. Liquid electrolytes, while inherently having high ionic conductivity, are comprised of lithium salts dissolved in flammable carbonate-based organic solvents. These highly flammable solvents, coupled with the concern for packaging derived from the leakage of these solvents, have become key issues for battery researchers. To alleviate these problems, research on electrolytes has been pervasive in both academia and industrial sectors. In this talk, I will briefly introduce our recent development of gel-state electrolytes utilizing silsesquioxane-based materials and ionic liquids. Silsesquioxanes, with chemical formula $[RSiO1.5]n$, provide a unique alternative to conventional polymer electrolytes, as the organic/inorganic functionality not only imbues non-leaking mechanical robustness, thermal stability, and high electrochemical stability, but also exhibits complete solution processability and unique ion transport behavior. Also, electrochemical performances of self-assembled ionic liquids crystal based ionogels will be discussed.

Symposium : **POLY2-2**
Recent Trends in Early-career Polymer Chemists
Room 402 (Live Streaming) TUE 13:55
Chair: Min Sang Kwon (Seoul National University)

Design and Synthesis of Reactive Polyolefin: Enabling Growth and Sustainability

Changwoo Nam

Jeonbuk National University, Korea

The objective of this research is to develop a practical and efficient oil recovery method that can be applied in large-scale crude oil spills in open water. The method is centered on a newly developed polyolefin oil superabsorbent, called “i-Petrogel”, in conjunction with existing mechanical (skimmer) recovery method. The i-Petrogel absorbent can be produced in large scale (>90 kg in our laboratory) by mixing two polyolefin polymers, including a semicrystalline linear low-density polyethylene (LLDPE) thermoplastic and a thermally cross-linkable poly(1-decene-co-divinylbenzene) (D-DVB) elastomer, to form an interpenetrated network structure with porous morphology. In two practical tests, i-Petrogel with a specific composition (LLDPE/D-DVB:1/1 weight ratio) shows selective absorption of Alaska North Slope crude oil on open water surface with fast kinetics and high absorption capacity of more than 40 times that of the polymer weight. In fact, i-Petrogel effectively stops the crude oil weathering process (evaporation, emulsification, and spreading) in open water. Furthermore, on the basis of our rheological findings on the resulting gel adducts, we propose that one can effectively recover these gels by a drum skimmer in both warm and cold conditions. The recovered oil/i-Petrogel adducts (hydrocarbons) contain almost no water, which can be refined as the original crude oil using regular refining processes (instead of chemical wastes). Overall, i-Petrogel technology potentially provides a comprehensive solution for combating crude oil spills in open waters, with dramatic reduction of environmental impact.

Symposium : **POLY2-3**
Recent Trends in Early-career Polymer Chemists
Room 402 (Live Streaming) TUE 14:20
Chair: Min Sang Kwon (Seoul National University)

Self-healing soft electronics: From materials to devices to system

Jiheong Kang

Department of Materials science and engineering, Korea Advanced Institute of Science and Technology, Korea

In recent years, considerable progress has been made in the development of self-healable materials. Despite significant progress, still self-healable materials have been rarely used for soft electronics due to their poor mechanical properties and incompatibility with other electronic materials. In this presentation I will first show my approaches to toughen self-healable network to use for soft electronic applications. Second I will talk about how to impart electronic functionalities to self-healable polymer network for integrated electronic skin applications. Finally, I will show explored opportunities in interconnection technologies in soft electronics by the use of self-healable materials. Through my presentation, I will cover from fundamental development of self-healing materials to their system level applications in soft electronics.

Symposium : **POLY2-4**
Recent Trends in Early-career Polymer Chemists
Room 402 (Live Streaming) TUE 14:45
Chair: Min Sang Kwon (Seoul National University)

Resin Functionalization with Protein N-Termini and Metal-Chelating Ligands

Byungjin Koo, Matthew Francis[1,*]

Department of Polymer Science and Engineering, Dankook University, Korea
[1]Chemistry, University of California, Berkeley, United States

Resin beads are granular crosslinked polymers. Their chemical modification has enabled scientific and industrial advances, such as combinatorial synthesis and the separation and purification of complex liquids. In this talk, two types of chemically modified resins are presented. First, we report functional proteins that are site-selectively immobilized on polymeric resin. Specifically, we employ an N-terminal protein modification strategy using an N-terminus-targeting reagent, 2-pyridinecarboxyaldehyde (2PCA), on resin through an imidazolidinone linkage. Seven different types of native proteins are N-terminally modified on resin with a high loading of proteins, and their utility to capture toxic hormones through protein-ligand interactions in water is underway. Second, polystyrene resin is functionalized with oligoethylene glycols (OEG). In spite of the widespread applications of ethylene glycol-type molecules, we found that the oligoethylene glycols can bind to lithium and cobalt with the different affinity. The mixture of lithium and cobalt in acetonitrile can be separated in a chromatographic column that is packed with the OEG-resin, and we envision that these materials can be used in the recycling of lithium ion batteries to extract metal components such as lithium and cobalt.

Symposium : **POLY3-1**
Recent Trends in the Development of Plastic Substrates
Room 402 (Live Streaming) TUE 15:10
Chair: Seokhoon Ahn (KIST)

Polyimide: Definition and Applications

Seung Woo Lee

School of Chemical Engineering, Yeungnam University, Korea

The physical and chemical behaviors of polymers are an extremely important area of research in polymer science. Polymer photochemistry has made extraordinary advances as a science during the last several decades. For flexible organic electronic device substrates, polymer materials should provide high gas barriers, flexibility, toughness and processability and desirable thermal and chemical properties. Of the many available polymeric materials, polyimides (PIs) have been widely used in the electronic device industry due to their high glass transition temperature, dimensional stability and heat resistance, as well as their excellent mechanical, adhesion and dielectric properties. The extraordinary properties of PIs come from strong intermolecular interaction through pi-pi interaction and charge transfer complex formation arising from used dianhydride and diamine monomers for polymerization. Nowadays, the development of photochromic polymers has become an active area of research. Several light sensitive chromophores like spiropyran groups are known for their important photoresponsive behaviors. When these chromophores become part of the polymer as pendant groups or in the polymer backbone, the photoresponsive behavior is induced to the polymers also. In this presentation, I will explain some thermal stable polymers and their application.

Symposium : **POLY3-2**
Recent Trends in the Development of Plastic Substrates
Room 402 (Live Streaming) TUE 15:35
Chair: Seokhoon Ahn (KIST)

Development of High performance polymers for plastic substrates

Nam-ho You

탄소융합소재연구센터, Korea Institute of Science and Technology, Korea

Aromatic polyimides (PIs) are one of the most important classes of advanced materials which possess various outstanding properties such as high thermal stability, chemical resistance, good mechanical and electric properties. Therefore, much attention has been devoted to aerospace, microelectronics, and optical device applications of PIs. We report an effective way to fabricate mechanically strong and multifunctional polyimide (PI) nanocomposites for plastic substrates. In this study, we will discuss general and effective strategies for the development of polyimide nanocomposite.

Symposium : **POLY3-3**
Recent Trends in the Development of Plastic Substrates
Room 402 (Live Streaming) TUE 16:00
Chair: Seokhoon Ahn (KIST)

Highly Stable Polyimide Dielectrics for High-performance Flexible Electronic Devices

Yun Ho Kim

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

Solution-processed organic field-effect transistors (OFETs) have many advantages in low-cost manufacturing, simple fabrication, and large-area processability over inorganic- and vacuum-processed FETs counterparts. To manufacture flexible electronic applications, their components must be mechanically flexible and durable. In particular, the thermally grown rigid inorganic gate insulators such as SiO2 and Al2O3 should be replaced with solution-processed organic gate insulators (OGIs) for large-area, low-cost, flexible electronics applications. Polymer insulators are promising candidates as gate dielectric layers in flexible OFETs due to their mechanical flexibility, solution processability, and low-temperature processability compared to inorganic gate dielectrics. Over the past two decades, various polymer materials including polystyrene (PS), poly(methyl methacrylate) (PMMA), polyvinylpyrrolidone (PVP), have been proposed as solution processed OGIs. Although flexible OFETs have been successfully implemented by many groups, there are still difficulties in actual commercialization because they cannot tolerate high process temperatures and in particular do not reach the insulation characteristics of inorganic insulators. Recently, polyimide (PI) has been attracting much attention as a gate dielectric material due to its remarkable thermal stability, chemical resistance, and mechanical flexibility. In this presentation, I will give an overview of PIs and present the results of a high-performance flexible OFETs using PI as a gate dielectric. In particular, I will focus on 1) soluble polyimides that can be processed at low temperatures and 2) water-soluble polyimides that are environmentally friendly.

Symposium : **POLY3-4**
Recent Trends in the Development of Plastic Substrates
Room 402 (Live Streaming) TUE 16:25
Chair: Seokhoon Ahn (KIST)

Mixed Ionic and Electronic Conduction in Radical Polymers

Yongho Joo

Advanced Functional Composite Materials Research Center, Korea Institute of Science and Technology, Korea

Organic mixed ionic and electronic conductors typically have heterogeneous conjugated macromolecular backbones and ether-based pendant groups to transport ions and charges. Moving from this archetype toward one with a single component, nonconjugated redox-active radical polymers that conduct both the charge and mass have significant benefits, such as they can be readily synthesized in large quantities and have the ability to produce either hole- or electron-transporting radical polymers by the selective tuning of the pedant group chemistry. Here, we demonstrate long-range (i.e., for lengths >50 μm) operational mixed ionic and electronic conduction in an amorphous, nonconjugated, low-glass-transition-temperature organic radical polymer upon blending the macromolecule with an ionic dopant lithium bis(trifluoromethanesulfonyl)imide salt (LiTFSI). Tuning the precise chemical nature of the functional radical pedant group using this ionic dopant is of key importance for the enhancement of long-range electrical conductivity. Moreover, the maximum ionic conductivity was 10^{-3} S cm^{-1} at elevated temperatures, and this was the highest reported value for a radical polymer-based system. Our findings demonstrate a significantly different macromolecular design paradigm than the commonly accepted heterogeneous composition for the creation of next-generation organic mixed ionic and electronic conductors.

Award Lecture in Division : **INOR1-5**
Organometallic Polymerization Catalysts
Room 401 (Live Streaming) TUE 11:00
Chair: Hoi Ri Moon (UNIST)

Photofunctionality of Transition Metal Complexes

Youngmin You

Chemical Engineering and Materials Science, Ewha Womans University, Korea

Cyclometalated complexes of d6 and d8 late transition metals offer unique merits for photoelectronic applications. The utility benefits from the strong orbital mixing between core metals and ligands and, also, from large spin-orbit coupling exerted by the metal center. To understand and create photofunction, I employ boundary-breaking techniques. Taking advantage of the strong phosphorescence emission, I have created molecular probes for visualization of endogenous species. The phosphorescent probes enable time-gated imaging of biospecimens. Synthetic modularity also permits the development of phosphorescent materials for use in organic light-emitting diodes. I recently discovered a new degradation mechanism of Ir(III) complexes which guides the design of highly stable electroluminescent compounds. The ability for utilization of triplet states has further been extended to photosensitization of biological singlet oxygen. This photofunction serves as a useful basis for photodynamic therapy. Finally, photoinduced one-electron transfer mediated by the complexes catalyzes a variety of organic transformations. Given the wide-ranging functionality, I believe that understanding and exploiting the photo(electrochemical) processes of inorganic molecules will significant broaden our horizons.

Award Lecture in Division : **INOR1-6**
Organometallic Polymerization Catalysts
Room 401 (Live Streaming) TUE 11:30
Chair: Hoi Ri Moon (UNIST)

Main Group Organometallic Complexes as Potential Optoelectronic Materials

Myung Hwan Park

Department of Chemical Education, Chungbuk Natioanl University, Korea

To date, numerous main group organometallic complexes based on group 13 metals, such as Al and Ga, have been widely reported as prominent optoelectronic materials due to their excellent electronic and photophysical properties. The luminescent properties of these complexes can be finely tuned in a strategic and systematic approach of the ligand frameworks. In particular, the introduction of various substituents into the ligand as a scaffold for organometallic complexes can induce fascinating photophysical properties, such as emission color tuning and quantum efficiency enhancement, leading to an expansion of their application as promising luminescent materials. In these perspectives, our group have recently developed various group 13-based aluminum and indium luminophores. On the basis of these recent results, we have found that the proper selection of both functional groups and a practical synthetic strategy can lead to attractive optical properties in these complexes. In this presentation, the details of the foregoing chemistry will be discussed.

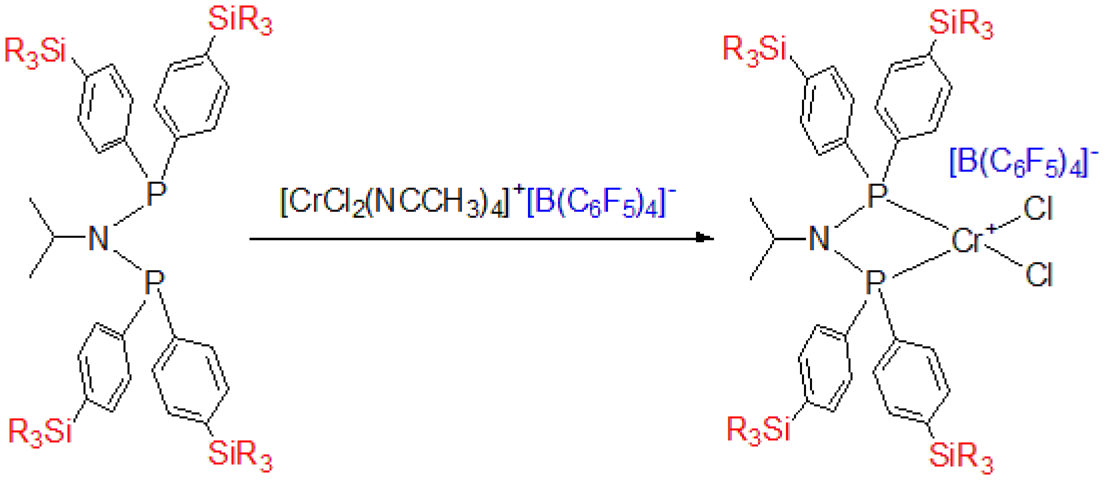
Symposium : **INOR1-1**
Organometallic Polymerization Catalysts
Room 401 (Live Streaming) TUE 09:00
Chair: Junseong Lee (Chonnam National University)

MAO-free Catalytic System for Ethylene Tetramerization

Bun Yeoul Lee

Department of Molecular Science and Technology, Ajou University, Korea

1-Octene is used as comonomers in the ethylene polymerization processes, and their demand has increased with the increase in the production capacity of linear low-density polyethylene (LLDPE) and polyolefin elastomer (POE). Cr-based catalysts that can selectively generate 1-hexene and/or 1-octene have been discovered. Cr-based catalytic system that generates 1-octene as the main product was also discovered at Sasol in the early 2000s. The original Sasol tetramerization catalyst is composed of Cr(acac)3, iPrN(PPh2)2 (abbreviated as PNP ligand), and expensive modified-methylaluminoxane (MMAO), which works best at a relatively low temperature of 60 °C. In large scale commercial operations with the original Sasol system, the use of expensive MMAO in excess (Al/Cr, ~500) is an economic disadvantage. Even though the reported activity of the typical Sasol system calculated based on Cr was extremely high (1200 kg/g-Cr), the productivity calculated based on the feed amount of MMAO was unsatisfactory (~2.0 kg/g-MMAO). Consequently, attempts have been made to replace expensive MMAO with inexpensive iBu3Al or Et3Al in combination with a stoichiometric amount of discrete non-coordinating anions (e.g., [Ph3C]+[B(C6F5)4]– or [PhN(H)Me2]+[B(C6F5)4]–). However, most of these attempts, especially with commonly used [Ph3C]+[B(C6F5)4]– and [PhN(H)Me2]+[B(C6F5)4]–, have been unsuccessful. In this study, we report an extremely active catalytic system that works with common trialkylaluminum iBu3Al avoiding the use of expensive MAO.


R3Si
SiR3
P
N
P
R3Si
SiR3
[CrCl2(NCCH3)4]+[B(C6F5)4]-
R3Si
SiR3
[B(C6F5)4]-
P
N
Cr+
Cl
Cl
P
R3Si
SiR3

Symposium : **INOR1-2**

Organometallic Polymerization Catalysts

Room 401 (Live Streaming) TUE 09:30

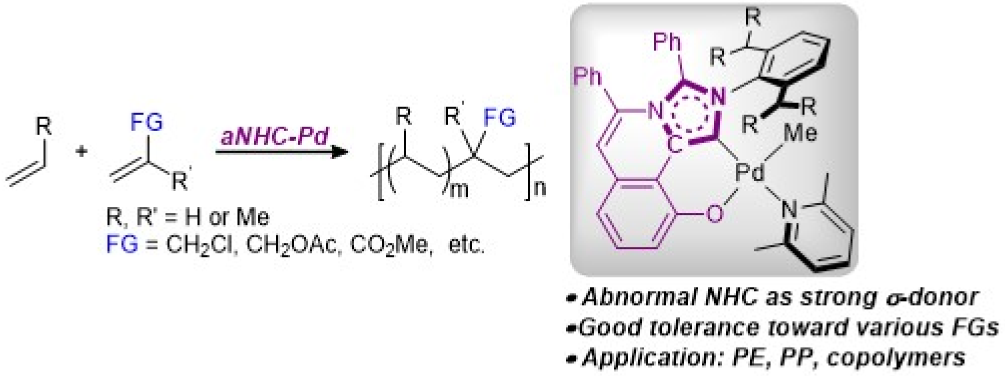
Chair: Junseong Lee (Chonnam National University)

Abnormal N-Heterocyclic Carbene Palladium Catalysts for the Copolymerization of Ethylene and Polar Monomers

Sukwon Hong

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

Palladium complexes bearing abnormal imidazo[1,5-a]pyridine-based N-heterocyclic carbene ligands (aImPy) were developed for the homopolymerization of olefins and the copolymerization of olefins and polar monomers. The highly electron-donating nature of these abnormal N-heterocyclic carbenes (aNHCs) embedded in the carbene-phenolate chelating ligand scaffold resulted in good catalytic activity, generating linear polyethylene with a high molecular weight (Mn = 237,000). aImPy-Pd complexes efficiently catalyzed propylene polymerization to afford polypropylene free of regio-defects. These catalytic systems exhibit good tolerance of various polar monomers and afford the desired copolymers. Up to 3.0% of the polar monomers were incorporated into the main chain, as determined by 1H and 13C NMR analysis. Furthermore, methyl methacrylate (MMA), as a 1,1-disubstituted ethylene derivative, was successfully incorporated into the main chain of polyethylene.



R, R' = H or Me
FG = CH_2Cl, CH_2OAc, CO_2Me, etc.

- *Abnormal NHC as strong σ-donor*
- *Good tolerance toward various FGs*
- *Application: PE, PP, copolymers*

Symposium : **INOR1-3**
Organometallic Polymerization Catalysts
Room 401 (Live Streaming) TUE 10:00
Chair: Junseong Lee (Chonnam National University)

Indol-2-ylidene (INDY): New Generation of N-heterocyclic Carbene with Facile Tunability and Scalability for Organic Synthesis

Eunsung Lee

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

Cyclic (alkyl)(amino)carbenes (cAACs) have attracted much attention since cAAC can effectively stabilize the unstable transition metal and main-group complexes through their strong σ-donating and appropriate π-accepting properties. Thanks to their remarkable stabilization effects, they could be successfully applied for the development of emissive materials and various catalytic reactions. However, there is a limitation for the electronic tunability of cAACs while their steric tunability was successful. To overcome the electronic tunability of cAAC, we designed a new N-heterocyclic carbene, indol-2-ylidene (INDY). INDY is an improved cAAC with an aryl backbone, which allows for the easy control of their electrical properties, rather than the existing saturated alkyl backbone of cAAC. Furthermore, indole, which is the basic skeleton of INDY, is ubiquitous in nature. Therefore, a large number of organic reactions have already been developed to synthesize various indole derivatives, which facilitates the synthesis of INDY derivatives, including various functional groups. The detailed synthetic methods and their application will be presented.

Symposium : **INOR1-4**
Organometallic Polymerization Catalysts
Room 401 (Live Streaming) TUE 10:30
Chair: Junseong Lee (Chonnam National University)

Homogeneous Catalysis for Polymerization of Methyl Methacrylate

Hyosun Lee

Department of Chemistry, Kyungpook National University, Korea

We have investigated catalytic activity for the polymerisation of methyl methacrylate (MMA) in the presence of catalysts transition metal complexes and co-catalyst modified methylaluminoxane (MMAO). Specifically, N,N'-bidentate or N,N',N-tridentate N’-substituted N,N-bis[(1H-pyrazol-1-yl)methyl]amines have applied to the transition metals such as cobalt, copper, zinc, and cadmium, to give a series of the corresponding transition metal complexes. All complexes were characterized by spectroscopic methods including X-ray crystallography. The MMA polymerization proceeds through an addition mechanism to give the activity as the order of 10^5 (g PMMA)/(mol cat)·h at 60°C and syndiotacticity of poly(methylmethacrylate) (PMMA), characterised by 1H NMR spectroscopy, was ca. 0.73.

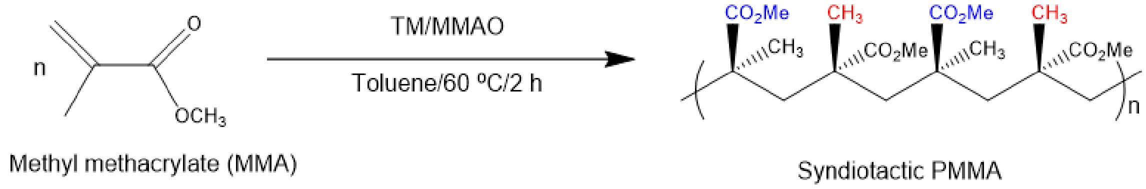


Figure 1. The polymerization of MMA

Symposium : **INOR2-1**

Probing Bioinorganic Chemistry: Imaging Bioinorganic Species

Room 401 (Live Streaming) TUE 13:00

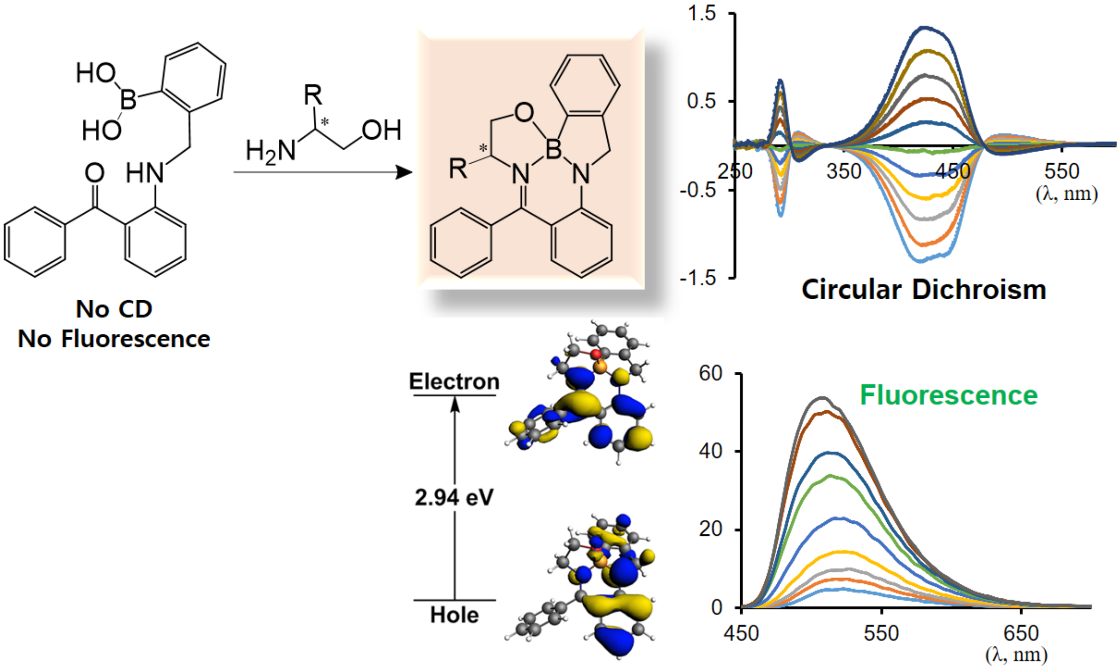
Chair: Youngmin You (Ewha Womans University)

Fluorescent imaging of inorganic Zn(II), biomolecules, and replacement of antibody with small molecules

Kwan mook Kim

Department of Chemistry, Ewha Womans University, Korea

Chiral aminoalcohols are important building blocks in the synthesis of pharmaceuticals and catalysts that play significant roles in biological processes, and they are used as markers for several diseases. Thus, sensors with the capability of determining the identity and ee of aminoalcohols are highly desirable in a variety of research areas. The derivatives of ortho-aminomethylphenylboronic acid and ortho-formylphenylboronic acid were reported as fluorescent probes for diols and as CD probes for aminoalcohols, respectively. Inspired by these studies, we designed compound 1, a diphenylketone moiety with an aminophenylboronic acid unit, which was proved to be a probe that gives both CD and fluorescence signals, allowing for convenient sensing of even aliphatic aminoalcohols which do not have any chromophores. This probe was observed to bind and image HSA protein selectively, which may further developed for small molecule replacing antibody. Here a probe that selectively imaging inorganic Zn(II) will be presented.


HO
B
HO
O
HN
No CD
No Fluorescence
R
*
H_2N
OH
R
*
O
B
N
N
1.5
0.5
-0.5
-1.5
250
350
450
550
(λ, nm)
Circular Dichroism
Electron
2.94 eV
Hole
60
40
20
0
450
550
650
(λ, nm)
Fluorescence

Symposium : **INOR2-2**

Probing Bioinorganic Chemistry: Imaging Bioinorganic Species

Room 401 (Live Streaming) TUE 13:25

Chair: Youngmin You (Ewha Womans University)

Scalable Surface-Enhanced Raman Scattering Nanoprobes for Biosensing and Bioimaging Applications

Jwa-Min Nam

Department of Chemistry, Seoul National University, Korea

Designing, synthesizing and controlling plasmonic metal nanostructures with high precision and high yield are of paramount importance in optics, nanoscience, chemistry, materials science, energy and biotechnology. In particular, synthesizing and utilizing plasmonic nanostructures with ultrastrong, controllable and quantifiable signals is key to the wide and practical use of plasmonic enhancement-based spectroscopies including surface-enhanced Raman scattering (SERS), but highly challenging. Here, I will introduce the design and synthetic strategies for molecularly tunable and structurally reproducible plasmonic nanogap structures with strong, controllable and quantifiable SERS or surface-enhanced fluorescence signals. I will also show their potentials in addressing some of important challenges in science, and discuss how these new plasmonic nanogap materials can lead us to new breakthroughs in biotechnologies including biosensing, bioimaging, theranostic and biocomputing applications.

Symposium : **INOR2-3**
Probing Bioinorganic Chemistry: Imaging Bioinorganic Species
Room 401 (Live Streaming) TUE 13:50
Chair: Youngmin You (Ewha Womans University)

Chemical Tools and Tactics to Study Multiple Facets in Alzheimer's Disease

Mi Hee Lim

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

Alzheimer's disease (AD), associated with degeneration of neurons and synapses in the brain, leads to motor impairment and eventual fatality. Neurodegeneration could be related to various interconnected features, including (i) plaque formation from amyloid-β (Aβ) peptide fragments, (ii) metal ion dyshomeostasis and miscompartmentalization, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). The inter-relations between some of these pathological factors have been investigated. Metals are found entangled in the Aβ plaque and likely contribute to Aβ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of Aβ plaque formation. Our understanding of the correlation between these elements and AD neuropathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease.[1-6] To find a cure for AD, we require a better understanding of the relationship between the various causative factors of this devastating disease. Towards this goal, we need suitable chemical tools capable of targeting and regulating its multiple underlying factors simultaneously.[2-4,6] Herein, our rational design and preparation of our chemical tools will be discussed with our investigations of their interactions and reactivities with targets *in vitro* as well as their efficacy *in vivo*.[7-14]

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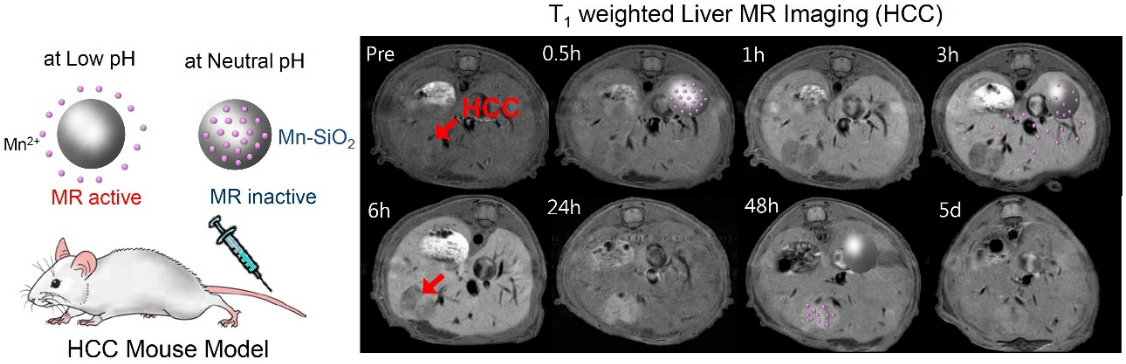
Symposium : **INOR2-4**
Probing Bioinorganic Chemistry: Imaging Bioinorganic Species
Room 401 (Live Streaming) TUE 14:15
Chair: Youngmin You (Ewha Womans University)

Liver Specific MRI Contrast Agents Based on Mn2+ Containing Nanoparticles

In Su Lee

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

In this presentation, I will discuss our strategy of developing Gd3+-free (low toxicity) contrast agents for liver MRI with high contrast-enhancing efficiency in T1-weighted MRI and lesion differential dynamic MR imaging properties, based on Mn2+-containing nanoparticles such as Mn2+-doped silica nanoparticle (Mn-SiO2) and hollow manganese silicate nanoparticle (HMS), by exploiting the characteristics of nanoparticles and cell-specific uptake and diffusion of released Mn2+ ions. Especially, I would like to demonstrate HMS, which exerts outburst-release of Mn2+ in the acidic physiological condition (e.g., endosomal solution of the Kupffer cell), as a liver-specific MR contrast agent with a high effectiveness in characterizing hepatic tumors, which was evaluated through the in-depth in-vivo MR imaging study and histochemical investigations. Time-sequential enhancement changes of three hepatic tumor models (e.g., hepatocellular carcinoma, neuroendocrine carcinoma, colonic adenocarcinoma) on the T1-weighted MR images after the HMS injection demonstrated their own characteristic contrast enhancement patterns, which reflect their biological features (e.g. tumor vascularity, cell density, mitochondrial activity, and hepatocellular specificity) and thus allows the disease-specific characterization of various hepatic tumors. Moreover, the investigation with hepatic artery-ligated tumor models mitochondrial activity proved the HMS-enhanced MR imaging to be effective in evaluating the extent of tumor necrosis in non-surgically treated hepatic tumors. Therefore, the use of HMS has the potential not only to replace arterial phase and hepatobiliary phase MR imaging using Gd-EOD-DTPA, due to its superior capability to diagnose an individual hepatic tumor specifically, but also to predict the therapeutic response of various hepatic tumors after non-surgical treatment.


T1 weighted Liver MR Imaging (HCC)
at Low pH
at Neutral pH
Mn2+
Mn-SiO2
MR active
MR inactive
HCC Mouse Model
Pre
HCC
0.5h
1h
3h
6h
24h
48h
5d

Symposium : **INOR2-5**
Probing Bioinorganic Chemistry: Imaging Bioinorganic Species
Room 401 (Live Streaming) TUE 14:40
Chair: Youngmin You (Ewha Womans University)

Development of Self-Assembled Nanostructures and Their Application

Ji Ha Lee

Department of Chemical Engineering, Hiroshima University, Japan

Supramolecular gels constitute a solid-like metal ion and bridging organic ligand structures that form multi-dimensional networks through a trapped solvent via non-covalent interactions. While physical properties of supramolecular gels show weak mechanical property comparing to conventional high molecular weight organic polymer gels, these gel systems are reversible and can be assembled/disassembled in the presence of added energy (i.e. heat, sonication, shaking, UV) to give a solution of gelator in solvent, or the gelled form. The solid/liquid nature of gels allow for species to migrate through the gel system interacting with metals, ligands, and the solvent. Chemosensing, catalysis, fluorescence, and drug-delivery applications are some of the many potential uses for these dynamic systems. In this symposium, I will introduce various types of supramolecular gels and their application as sensors based on fluorescence properties which appear when molecules are self-assembled.

Symposium : **INOR3-1**
Recent Research Trends in Soli-State Chemistry and Metal Complex Chemistry
Room 401 (Live Streaming) TUE 15:00
Chair: Tae-Soo You (Chungbuk Natioanl University)

Phase Boundary Mapping Thermoelectric Semiconductors

G Jeffrey Snyder

Materials Science, Northwestern University, United States

We often understand the physical properties of Zintl Phases by considering the perfect crystalline material that is defect free. Yet this perfect, stoichiometric (valence balanced) crystal is an intrinsic semiconductor with equal number of electrons and holes. To make a n-type or p-type semiconductor we typically use point defects to introduce a slight valence imbalance that leads to excess electrons or holes. Often intrinsic defects such as vacancies, interstials or antisite defects, provide the necessary carriers to make the material a good thermoelectric (e.g. Zn4Sb3, Bi2Te3-Sb2Te3, YbxCoSb3, etc.). Most materials, however, require extrinsic dopants to be a good thermoelectric and intrinsic defects only make it more complicated. Sometimes intrinsic defects are so prevalent they are killer defects that prevent any dopant from making the material n-type or p-type. By understanding that atomic chemical potentials influence defect energy and also define regions in phase diagrams we can use phase boundary mapping to explore all the possible thermodynamic defect states of a material to avoid killer defects. The most dramatic demonstration of this is the discovery of high zT n-type Mg3Sb2 which only occurs in Mg-rich Mg3Sb2 where Mg-vacancies are suppressed.Point defects can also make gradual but profound changes to the band structure compared to the defect free compound. This includes increasing band gap for higher temperature application, reducing conductivity mass for higher mobility or band convergence for dramatic increase in density of states (Pb(Se,Te), Mg2(Si,Sn), Bi2Te3-Sb2Te3,). In principle all of these defects can be better controlled by engineering chemical potentials through phase boundaries. Even the Ni content MNiSn (M = Ti, Zr, Hf) Half-Heusler thermoelectrics can be sufficiently altered to make substantial differences in electronic properties. The excess Ni produces impurity states in the band gap that changes the effective band gap and leads to additional electron and phonon scattering.References[1] Ohno, Snyder et al, Joule 1, 141 (2018)[2] Gregory S. Pomrehn, Alex Zevalkink, W. G. Zeier, A. van de Walle and G. J. Snyder “Defect controlled electronic properties in AZn2Sb2 Zintl phases (A=Ca, Sr, Eu, Yb)”, Angewandte Chemistry, 126, 3490 (2014)[3] Yinglu Tang, S-W Chen, G. J Snyder “Temperature Dependent Solubility of Yb in Yb-CoSb3

Skutterudite and its Effect on Preparation, Optimization and Lifetime of Thermoelectrics“ Journal of Materiomics 1, 75 (2015)[4] Alex Zevalkink, Gregory S. Pomrehn, Samantha Johnson, Jessica Swallow, Zachary M. Gibbs, and G. Jeffrey Snyder “Influence of the triel elements (M = Al, Ga, In) on the transport properties of Ca5M2Sb6 Zintl compounds” Chem. Mater 24, 2091 (2012)[5] Gregory S. Pomrehn, Alex Zevalkink, Wolfgang G. Zeier, Axel van de Walle and G. Jeffrey Snyder “Defect controlled electronic properties in AZn2Sb2 Zintl phases (A=Ca, Sr, Eu, Yb)”, Angewandte Chemistry, 126, 3490 (2014)

Symposium : **INOR3-2**
Recent Research Trends in Soli-State Chemistry and Metal Complex Chemistry
Room 401 (Live Streaming) TUE 15:25
Chair: Tae-Soo You (Chungbuk Natioanl University)

Metal Alloy Nanoparticles with Controlled Shell Thickness of Noble Metals for Catalysis

Won Seok Seo

Department of Chemistry, Sogang University, Korea

Metal alloy nanoparticles composed of a noble metal and a first-row transition metal are of great interest for technological applications such as fuel cells based on hydrogen and small organic molecules, catalysts toward the hydrogen evolution reaction and hydrogenation reaction, and sensors, because such nanoparticles utilize less amounts of the precious noble metal and exhibit enhanced catalytic or electrocatalytic properties, including high activity, selectivity, and durability. Most recent efforts have focused on improving the Pt efficiency of Pt-based alloy nanoparticles by controlling their composition, morphology, and structure. Among various Pt-based alloy nanoparticles, FePt nanoparticles have been demonstrated to be more efficient than pure Pt nanoparticles in catalyzing electrochemical reactions such as CO oxidation, methanol oxidation, and oxygen reduction. The incorporation of Fe not only reduces the Pt content of Pt-based electrocatalysts but also dramatically increases their catalytic activities by lowering the Pt d-band structure and providing suitable Pt atom compression on the catalyst surface. In the presentation, I will introduce metal alloy nanoparticles with controlled shell thickness of noble metals developed by our group and their catalyst applications toward the methanol oxidation, hydrogen evolution, and hydrogenation reactions.

Symposium : **INOR3-3**
Recent Research Trends in Soli-State Chemistry and Metal Complex Chemistry
Room 401 (Live Streaming) TUE 15:50
Chair: Tae-Soo You (Chungbuk Natioanl University)

Chemical Reactions on Surfaces: Fabrication of Nanostructured Surfaces and Their Applications

Jin Seok Lee

Department of Chemistry, Hanyang University, Korea

Nanotechnology makes it possible to intentionally modify the properties of surfaces and endow them with any desired function. Nanostructured surfaces have represented important advances in control of wetting, adhesion, and mechanical, thermal, magnetic, electrical, and optical properties and ability to direct cell behavior. A number of promising approaches to fabricate functional micro- and nanostructured surfaces have been stimulated by opportunities to enhance the properties of surfaces and interfaces via the combination of surface structure, morphology, and physical and chemical properties. Such functional micro- and nanostructured surfaces are playing an increasingly important part in a broad range of novel applications, such as energy, electronics, photonics, as well as sensor systems, advanced materials, and medical devices.In this presentation, I will introduce our recent experimental results based on chemical reactions on solid surfaces, which are fabrications of nanostructured surfaces including vertically aligned Si nanowire arrays, closely packed beads, and porous anodic alumina. Also, I will discuss various surface treatment techniques, such as molecular layer deposition and liquid phase deposition, with the aim of improving their surface properties and functional performance, as well as new insights on physical principles underlying their properties and enormous potential applications.

Symposium : **INOR3-4**

Recent Research Trends in Soli-State Chemistry and Metal Complex Chemistry

Room 401 (Live Streaming) TUE 16:15

Chair: Tae-Soo You (Chungbuk Natioanl University)

Multifunctional Core-shell Pd@Cu on MoS_2 as a Visible Light-harvesting Photocatalyst for Synthesis of Disulfide by S-S Coupling

Kang Hyun Park

Department of Chemistry, Pusan National University, Korea

Visible light harvesting materials are considered promising cost-effective heterogenous catalysts for organic synthesis. A novel and efficient synthesis of multifunctional core-shell Pd@Cu/MoS_2 nanostructures is utilized for synthesis of disulfides by S-S Coupling. The Pd@Cu core-shell was obtained by one-pot hydrothermal synthesis, and a simple method was used to load it onto the MoS_2. The as-prepared materials were characterized by scanning electron microscopy, transmission electron microscopy, X-ray powder diffraction, N_2 sorption isotherms, X-ray photoelectron spectroscopy, UV-vis diffuse reflectance spectroscopy, and photoluminescence spectroscopy. The Pd@Cu/MoS_2 nanostructures revealed excellent photocatalytic activity, reusability, and stability towards the oxidative coupling of mercaptans to disulfanes. The outstanding photocatalytic activity of Pd@Cu/MoS_2 will enhance interest in the field of multifunctional core-shell nanomaterials as photocatalysts for a wide variety of applications.

Symposium : **INOR3-5**

Recent Research Trends in Soli-State Chemistry and Metal Complex Chemistry

Room 401 (Live Streaming) TUE 16:40

Chair: Tae-Soo You (Chungbuk Natioanl University)

Metal-Ion Doped Semiconductor Photocatalysts for Photocatalytic Hydrogen Evolution Reaction

Jong Wook Hong

Chemistry, University of Ulsan, Korea

Solar energy conversion systems have attracted intense attention as clean, sustainable, and environmentally friendly energy sources. A wide spectrum of photoactive materials, ranging from organic dyes to semiconductors, has been explored for efficient light absorption and photogenerated charge transfer. Recently, surface-modified semiconductors have recently led the rapid progress in enhancing photocatalytic efficiency under visible light irradiation, including the aspects for environmental and energy applications such as CO2 conversion, water splitting, and pollutant treatment. However, its practical application is limited due to low light harvesting efficiency, fast charge recombination, and low stability of current photocatalysts. Herein, we introduce high-performance solar energy conversion platforms constructed by doping metal ions dopants into semiconductor photocatalysts (InP@ZnS QDs and CdS-P nanorods). The metal ions doped on prepared photocatalysts show efficient electron/hole capturing capability, which increase the electron/hole transfer efficiency through retardation of charge recombination. Therefore, the photocatalysts showed outstanding hydrogen evolution performances under visible-light irradiation compared with their counterparts. The prepared photocatalysts could enable the drastic elevation of solar energy conversion efficiency as well as the elucidation of the underpinning mechanism of surface metal ion mediated photocatalysis.

Award Lecture in Division : **PHYS1-1**
Recent Methodologies in Biomolecular Spectroscopy
Room 403 (Live Streaming) TUE 10:40
Chair: Han Bin Oh (Sogang University)

Reaction Dynamics of Photofunctional Molecules by Ultrafast X-ray Spectroscopy

Tae Kyu Kim

Department of Chemistry, Yonsei University, Korea

The geometrical structures of molecular species during chemical reactions as well as relevant electronic configurations and spin-states are crucial information on understanding various photochemical and photobiological processes. For this purpose, time-resolved X-ray spectroscopy has been developed as a complimentary tool for the ultrafast optical spectroscopies. Essentially, due to the element-specific valence-to-core level transition of probing X-rays, time-resolved X-ray spectroscopy can be sensitive spectral probes of metal-ligand interactions of solvated transition metal complexes. We have focused on these element-specific probing natures of X-ray pulses and elucidated structural dynamics in several important classes of transition metal complexes. In this presentation, I will describe our recent works on the ultrafast linkage isomerization of Ru-based photochromic complex. More specifically, we have utilized Ru L-edge and S K-edge X-ray spectroscopies to unravel details of excited state dynamics. X-ray spectra reveal the spin and valence charge of the Ru atom and provide experimental evidence that metal-centered excited states mediate isomerization. Complementary X-ray spectra of the functional ligand S atoms probe the nuclear structural rearrangements, highlighting the formation of two metal-centered states with different metal-ligand bonding. Our results address an essential open question regarding the relative roles of transient charge-transfer and metal-centered states in mediating photoisomerization.

Award Lecture in Division : **PHYS1-2**
Recent Methodologies in Biomolecular Spectroscopy
Room 403 (Live Streaming) TUE 11:05
Chair: Han Bin Oh (Sogang University)

Automated prediction of chemical reactions

Woo youn Kim

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

Despite remarkable advances in computational chemistry, the prediction of chemical reactions is still challenging, because investigating possible reaction pathways is computationally prohibitive due to the high complexity of chemical space. For instance, their brute-force sampling is too demanding because of their large degrees of freedom. A stochastic sampling method inherently requires many trials no matter how effective it is, because it cannot guarantee a 100% probability of finding a designated target structure within a finite number of samplings. A feasible strategy for efficient prediction is to utilize chemical heuristics and machine learning techniques. We proposed a novel approach to search reaction paths in a fully automated fashion by combining chemical theory and heuristics. A key idea of our method is to extract a minimal reaction network composed of only favorable reaction pathways from the complex chemical space through molecular graph and reaction network analysis. This can be done very efficiently by exploring the routes connecting reactants and products with minimum dissociation and formation of bonds. Finally, the resulting minimal network is subjected to quantum chemical calculations to determine kinetically the most favorable reaction path at the prediction accuracy. To further accelerate the graph-based method, we introduce state-of-the-art machine learning techniques. They can replace chemical heuristics and expensive calculations with more systematic, unbiased computational rules. In this talk, we show the recent progress in this project with several examples.

Symposium : **PHYS1-3**
Recent Methodologies in Biomolecular Spectroscopy
Room 403 (Live Streaming) TUE 11:30
Chair: Jung Ho Lee (Seoul National University)

Time-Resolved X-ray Tools to Study Protein Dynamics

Hyotcherl Ihee

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

Time-resolved x-ray liquidography (TRXL), which is also known as time-resolved x-ray solution scattering, has been successfully used to reveal the structural dynamics of various biological reactions [1-7] as well as small molecules [8-10]. The characteristic of x-ray, of which scattering signal is sensitive to the global structures of proteins, allows for visualizing the global structural changes of proteins during reactions. We will present up-to-date TRXL experiments and analysis results for protein folding and signal transition within a protein. In addition, we will present our recent development to make TRXL applicable to a wider range of proteins. We expect that such experimental enhancements could extend the application of TRXL to an unprecedented realm in terms of their target proteins and time domain.[1] Nat. Methods, 5, 881-887 (2008)[2] Acc. Chem. Res., 48, 2200-2208 (2015)[3] Proc. Natl. Acad. Sci., 117, 14996-15005 (2020)[4] J. Phys. Chem. B, 124, 1550-1556 (2020)[5] Int. J. Mol. Sci., 19, 3633 (2018)[6] J. Am. Chem. Soc., 134, 3145-3153 (2012)[7] J. Am. Chem. Soc., 134, 7001-7008 (2012)[8] Science, 309, 1223-1227 (2005)[9] Nature, 518, 385-389 (2015)[10] Nature, 582, 520-524 (2020)

Symposium : **PHYS1-4**
Recent Methodologies in Biomolecular Spectroscopy
Room 403 (Live Streaming) TUE 11:50
Chair: Jung Ho Lee (Seoul National University)

Exchangeable Probes for Bleaching-resistant Single-molecule Localization Microscopy

Sang-Hee Shim

Department of Chemistry, Korea University, Korea

Single-molecule localization microscopy (SMLM) reconstructs super-resolution images by accumulating precisely localized centroid positions of many fluorophores. The spatial resolution, the highest among various super-resolution methods, is determined by both the precision and density of localization points (i.e. centroid positions of single molecules). While the localization precision has been improved up to sub-10-nm by developing high-photon probes (as in DNA-PAINT) as well as high-precision localization techniques (as in MINFLUX), the localization density is limited by photobleaching involved with permanent, chemical damage of fluorophores. We overcome the photobleaching limit by uncovering new chemistry and classes of exchangable probes whose association and dissociation cycles replace bleached fluorophores with fresh probes in solution. DNA-PAINT suffers from high fluorescent background from unbound fluorescent probes that substantially slow down the imaging speed. We chemically reduce DNA-PAINT probes into a nonfluorescent state and improve the imaging speed up to two orders of magnitude. For live-cell imaging that requires genetically encodable exchangeable probe, we introduce UnaG, a ligand-activatable fluorescent protein capable of reversible fluorescence recovery that allow for high localization density lasting for a long imaging period. By combining UnaG with CRISPR imaging, we capture live-cell movie of chromatin structures composed of hundreds of super-resolution frames. We anticipate that super-resolution movies of genomic loci will unveil the chromatin structures and dynamics in individual cells that may reflect different states of the cell or the local nuclear environment.

Symposium : **PHYS1-5**
Recent Methodologies in Biomolecular Spectroscopy
Room 403 (Live Streaming) TUE 12:10
Chair: Jung Ho Lee (Seoul National University)

Binuclear Activation of O2 – Spectroscopic Elucidation of Intermediates

Kiyoung Park

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

O2 is known to be the most benign and cheap oxidant, but its paramagnetic nature disallows a direct reaction with diamagnetic organic substrates. Nature activates O2 by employing metalloenzymes, the active sites of which contain transition metal cofactors and thus can transfer a single electron to reduce O2. The O2-to-superoxide conversion though involves uphill thermodynamics; thus enzymes often employ another cofactor or another metal center to provide an additional electron to O2 so that exothermic peroxide formation occurs instead.Recently we have found that organonickel complexes can activate O2 in a similar manner that binuclear oxygenases utilize O2. Most organometallic catalysts that are widely utilized are incapable of activating O2 in a controlled way, while using O2 as an oxidant is desirable. A couple of Pd and Cu organometallic catalysts have been reported to use O2 as an oxidant. However, these reactions still require heating, and O2 simply uptakes electrons to form high-valent metal centers, in contrast to the metallo-oxygenases, where the oxygen atom of O2 can be incorporated to organic substrates. Our findings reveal that organonickel complexes can selectively either oxidize or oxygenate alkyl substrate depending on supporting ligands, showing reactivity parallel to monooxygenase enzymes. We have studied the electronic and geometric structures of intermediates in this reaction by employing various spectroscopic techniques that have been utilized to study metalloenzymes. This electronic-structure level understanding will provide key insights to broaden the O2 reactivity in organometallic chemistry.

Symposium : **PHYS1-6**
Recent Methodologies in Biomolecular Spectroscopy
Room 403 (Live Streaming) TUE 12:30
Chair: Jung Ho Lee (Seoul National University)

Elucidating Protein Topologies Using Ion Mobility-Mass Spectrometry: From String to Pretzelane

Jongcheol Seo

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

The protein topologies as well as structures, conformations are of great interest to the protein functions. Indeed, many different protein topologies are exist in nature, for example, a common linear string, a cyclic form, a threaded or extended lasso, a knotted or chained form and many more. Furthermore, an artificial proteins can be designed to have a specific topology, in order to engineer the protein functions. Thus, identifying and distinguishing such diverse topologies have a big significance for designing and characterizing such topologically-engineered proteins. In the present work, we implemented ion mobility-mass spectrometry (IM-MS) to investigate the topological as well as conformational transitions of specially-designed proteins (lasso-BXA) which can have a lasso topology. With IM-MS, we could distinguish different topologies and conformations of l-BXA, such as a threaded lasso and an extended tadpole, by measuring collision cross section values. Furthermore, transitions between threaded lasso and extended tadpole were observed upon collisional activation, which confirms the predicted topologies and conformations. Through this study, we have presented possibilities in examining the topological isomers of proteins with IM-MS. We expect this IM-MS approach may be established as a useful tool for studying protein topology.

Award Lecture in Division : **PHYS2-1**
Recent Physical Chemistry Studies on Photovoltaic Materials
Room 403 (Live Streaming) TUE 13:30
Chair: Han Bin Oh (Sogang University)

VUV-MATI spectroscopy towards conformational chemistry

Chan Ho Kwon

Department of Chemistry, Kangwon National University, Korea

In the symposium, I will introduce the cutting-edge mass spectroscopic techniques based on mass spectrometry and laser spectroscopy for study on the conformational structure of polyatomic molecule, along with the experimental results. An in-house built vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) mass spectrometer could routinely provide the high-resolution (~5 cm^{-1}) vibrational spectrum of molecular cation. Based on the vibrational potential energy surfaces constructed along the conformational coordinates at the density functional theory levels, the Franck-Condon analysis of the measured MATI spectrum elucidate the conformational structure of the molecular cation. Furthermore, to investigate the conformational structure of the corresponded neutral, the IR dip /VUV-MATI spectroscopy was exploited. Based on the fact that the IR absorption of a neutral conformer in the molecular beam results in the depletion of the 0-0 band in the VUV-MATI spectrum of the conformer, the dip in the 0-0 band signal recorded as a function of IR photon energy appears when the conformer is vibrationally excited by the IR, which provides the vibrational spectrum of the neutral conformer. Thereafter, the IR depletion /VUV-MATI spectroscopy was applied to obtain the vibrational spectrum of the cationic conformer. Based on the IR dip spectrum of the designated conformer, the IR absorption of the conformer reflects the depletion in the MATI intensities corresponded to the conformer, which ultimately provides the vibrational spectrum of the cationic designated conformer. These cutting-edge techniques will allow to study the conformational chemistry in numerous molecular systems.

Symposium : **PHYS2-2**

Recent Physical Chemistry Studies on Photovoltaic Materials

Room 403 (Live Streaming) TUE 14:00

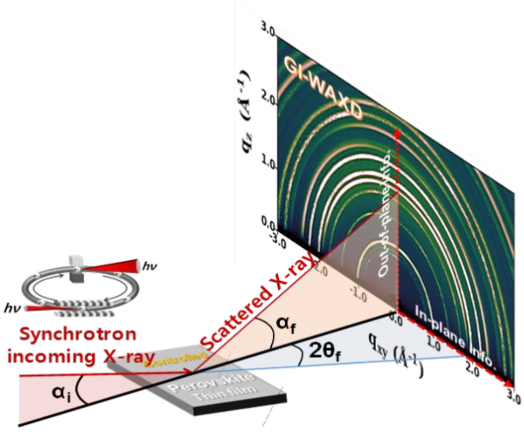
Chair: Myeongkee Park (Dong-A University)

Synchrotron radiation applications to study the structure-property relationship of halide perovskite materials

Tae Joo Shin

UCRF/Chemistry, Ulsan National Institute of Science and Technology, Korea

Recently, halide perovskite solar cells have achieved 25.2% photo-to-power conversion efficiency in small-sized cells [1], which has high expectation for commercialization. However, for the final commercialization of halide perovskite solar cells, manufacturing costs should be lowered, large area efficiency should be increased, and long-term stability against external environments (temperature, humidity, light illumination, and etc.) must be improved [2]. To meet these demands, detailed structural understanding of perovskite materials and structural changes according to external environment, design and synthesis of new materials based on these understandings, and other key layers (ETL, HTL, and etc.) that make up solar cells should be optimized. In this presentation, the basics and applications of various in-situ and ex-situ synchrotron X-ray experiments (XRD, GIXD, and XAFS) on halide perovskite thin films, which have recently received a lot of attention among energy conversion materials and numerous studies are actively being conducted, are introduced. In order to study the structure-property correlation of perovskite thin films, this study includes not only the structure at room temperature, but also at low and high temperature structure and phase transformation, the long-term storage behavior under atmospheric and vacuum condition, and the behavior under light irradiation. References: [1] NREL, Best Research-Cell Efficiency Chart, https://www.nrel.gov/pv/cell-efficiency.html. [2] Y. Rong et al., Science 361, eaat8235 (2018); G. Divitini et al., Nature Energy 1, 1-6 (2016); T. A. Berhe et al., Energy Environ. Sci., 9, 323 (2016); H. Zhang et al., Nat. Commun., 10, 1-8 (2019). Acknowledgement: This work was supported by NRF-2018R1A5A 1025224 and CAP-18-05-KAERI.


GI-WAXD
q_z (Å⁻¹)
3.0
2.0
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Out-of-plane info.
In-plane info.
q_xy (Å⁻¹)
hν
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Synchrotron
incoming X-ray
Scattered X-ray
α_f
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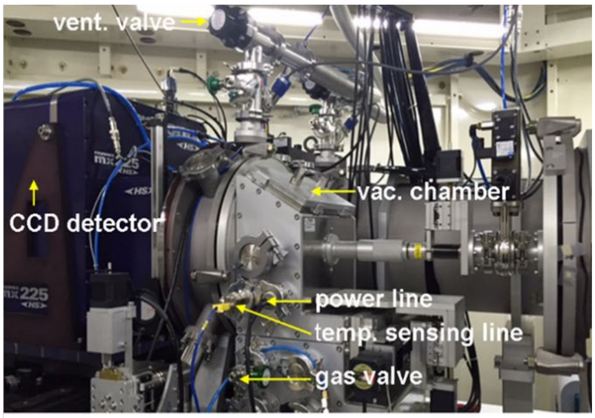
α_i
Perovskite
Thin film


vent. valve
vac. chamber
CCD detector
power line
temp. sensing line
gas valve

Symposium : **PHYS2-3**
Recent Physical Chemistry Studies on Photovoltaic Materials
Room 403 (Live Streaming) TUE 14:20
Chair: Myeongkee Park (Dong-A University)

Carrier Multiplication in Carbon-Based Nanosystems

Junhyeok Bang

Department of Physcis, Chungbuk Natioanl University, Korea

Carrier multiplication (CM) is a fundamental process of an excited carrier that generates multi-electron-hole pairs from a single photon absorption, and thus it can enhance optoelectronic device efficiency. However, CM is rather inefficient in conventional semiconductors because of strong restrictions imposed by the energy and momentum conservation. Here, using real-time time-dependent density functional theory, we show that CM occurs in carbon-based nanosystems due to the existence of subbands. The CM mechanism is different from the ones suggested for quantum dots and graphene. Furthermore, the band gap of the carbon-based nanosystem is significantly modulated depending on system size, and thus it provides the way to control the carrier dynamics and carrier multiplication.

Symposium : **PHYS2-4**
Recent Physical Chemistry Studies on Photovoltaic Materials
Room 403 (Live Streaming) TUE 14:40
Chair: Myeongkee Park (Dong-A University)

A strategy for reducing the trap density in halide perovskite solar cells

Hui-Seon Kim

Department of Chemistry, Inha University, Korea

Trap-assisted non-radiative recombination is a major source suppressing the performance in halide perovskite solar cells. In this study, strategies ranging from an artificial treatment with surface passivating agents to a photo-induced trap reduction at device operating condition are investigated. A mixture of a new ammonium salt, $CF_3(CF_2)_2CH_2NH_3I$ (HBAI), and a conventional formamidinium halide, FAX, is used for the surface passivation on top of the 3D perovskite bulk film. The employment of the passivation layer not only suppresses charge recombination by passivating the surface traps of the 3D perovskite film but also builds a well-matched energy alignment at the interface of perovskite/HTM, being attributed to the internal interaction between the agents. Notably, the passivation layer improves the long-term stability based on the decreased trap density as well as an increased moisture-resistance. On the other hand, the trap density of the device shows a gradual decrease near maximum power point (mpp). An increase in the photocurrent at mpp is accordingly observed owing to the reduced trap density. The beneficial charge-transfer properties of under illumination is addressed by relating to the photo-induced structural response of the perovskite.

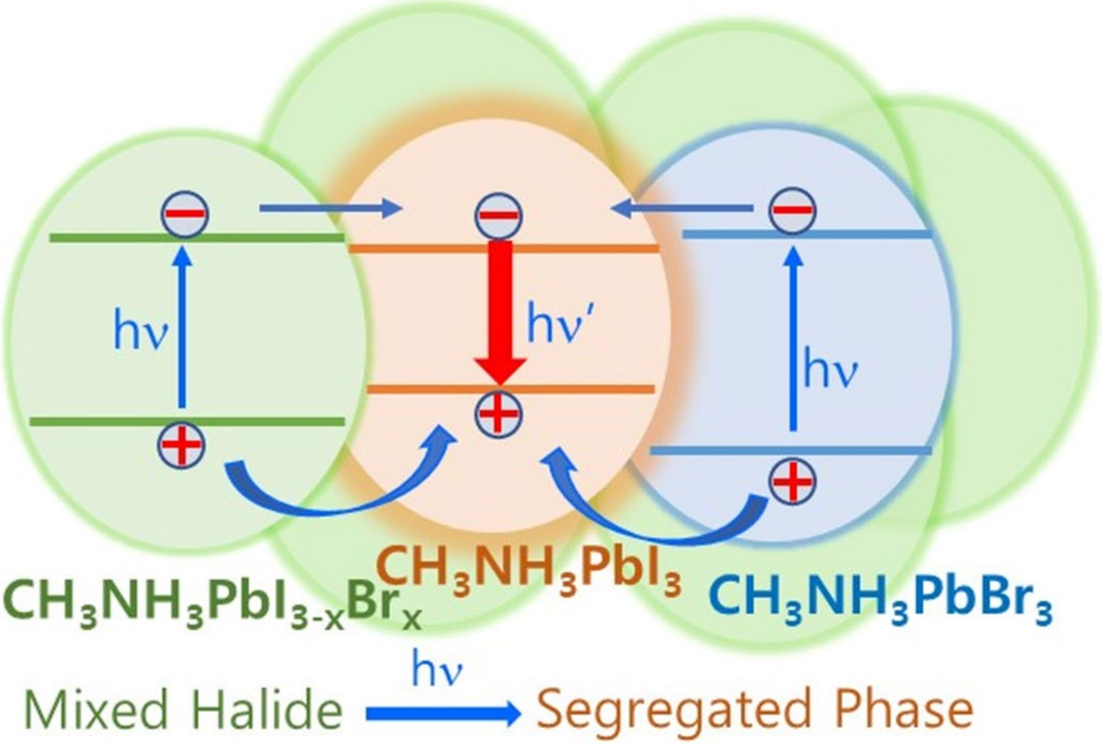
Symposium : **PHYS2-5**
Recent Physical Chemistry Studies on Photovoltaic Materials
Room 403 (Live Streaming) TUE 15:00
Chair: Myeongkee Park (Dong-A University)

Phase Segregation in Mixed Halide Perovskite: Fundamentals and Strategies to Obtain Photostability

ChaeHyun Lee, Soo Jeong Lee[1], YeJi Shin, YouJeong Lee, Seog Joon Yoon[2,*]

Yeungnam University, Korea
[1]*Chemistry, Yeungnam University, Korea*
[2]*Department of Chemistry, Yeungnam University, Korea*

Mixed halide perovskites are one of the promising candidates for solar cells, light-emitting diodes (LEDs), and other applications due to their tunable optical properties by varying halide compositions. To apply the mixed halide perovskite to the devices, it is essential to understand as follows: 1. fundamental photophysical properties, 2. photoinduced processes, 3. strategies to improve photostability, and 4. impact of interfacial recombination process to the solar cell performance. In this talk, 1. impact of halide-Pb complex to optical properties, 2. photoinduced reversible phase segregation process of mixed halide under short-term irradiation, 3. irreversible photodegradation process beyond the phase segregation under long-term irradiation, 4. strategies to obtain photostability, and 5. fundamental study about interfacial charge accumulation/recombination in the solar cell will be presented with various characterizations, such as absorption/emission/transient absorption spectroscopies, in-situ XPS, Kelvin probe force microscopy, and so on.


hν
hν′
hν
$CH_3NH_3PbI_{3-x}Br_x$
$CH_3NH_3PbI_3$
$CH_3NH_3PbBr_3$
hν
Mixed Halide
Segregated Phase

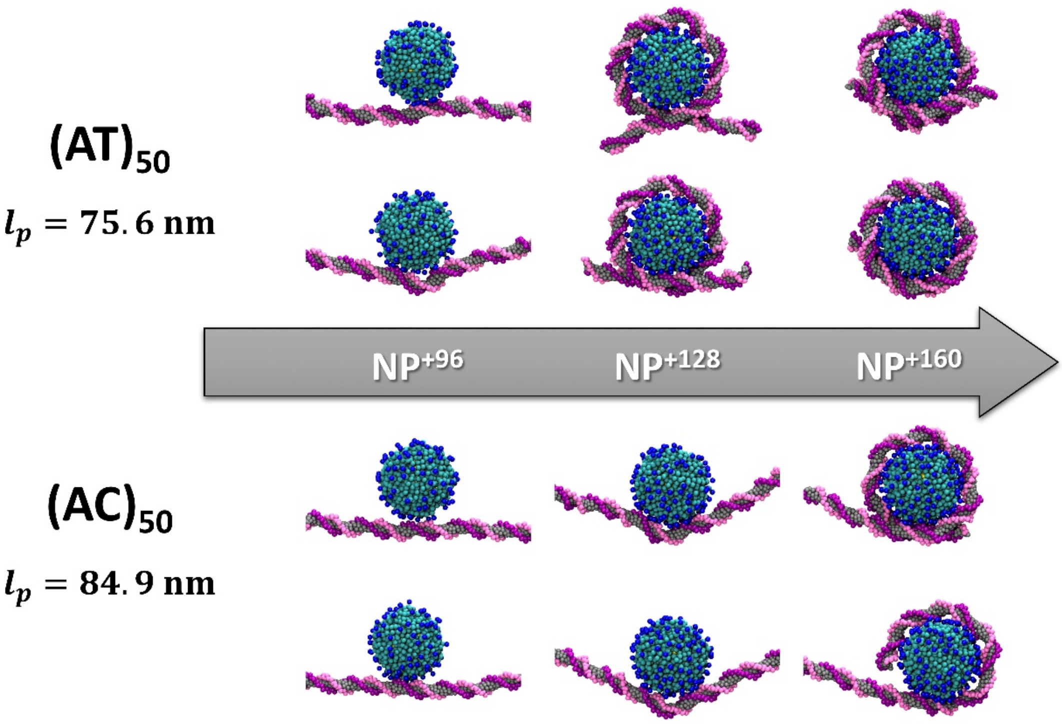
Symposium : **PHYS3-1**
Recent Theoretical and Computer Simulation Studies of Macromolecules
Room 403 (Live Streaming) TUE 15:30
Chair: Sanghun Lee (Gachon University)

Competition between electrostatic bending and intrinsic rigidity of DNA in binding with a cationic nanoparticle: towards the development of a Brownian motor

Jun Soo Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

We design a DNA-based Brownian motor for directional transport of positively charged nanoparticles along a single, long double-stranded DNA (dsDNA) with elaborately designed flexibility variation. To prove its realization, we first investigate the bending of intrinsically rigid dsDNA by binding with a cationic nanoparticle, using the coarse-grained molecular dynamics simulations. An electric charge of the nanoparticle and the sequence-dependent flexibility of dsDNA are varied to elucidate the competitive effects of intrinsic rigidity of dsDNA and electrostatic interactions between charged dsDNA and a nanoparticle. We prove that the nanoparticle wrapped around by dsDNA rolls over the dsDNA towards more flexible region of the dsDNA. This work suggests that dsDNA molecules with elaborately designed flexibility variation can be used as a molecule-scale guide for spatial and dynamic control of nanoparticles for future applications.


$(AT)_{50}$
$l_p = 75.6$ nm
NP^{+96}
NP^{+128}
NP^{+160}
$(AC)_{50}$
$l_p = 84.9$ nm

Symposium : **PHYS3-2**
Recent Theoretical and Computer Simulation Studies of Macromolecules
Room 403 (Live Streaming) TUE 15:50
Chair: Sanghun Lee (Gachon University)

Efficient simulation approach for prediction of phase separation and shape evolution in polymer solution assembly

Su-mi Hur

Chonnam National University, Korea

The self-assembly in various polymeric systems is the core principle of many advanced nanotechnologies. Theoretical and numerical studies have provided valuable insights into understanding the underlying physical principles in the self-assembly of polymeric systems and powerful tools and guidelines for designing experiments. Especially, coarse-grained fields- or particle- base models have successfully predicted equilibrium morphologies of self-assembled structures and have assisted in finding feasible ways to control the shape, size, and arrangement direction of self-assembled structures. However, often complicated interactions, non-flat free surface, high sensitivity on various system parameters, a wide range of length and time scales related to self-assembled structures prevent the usages of existing theoretical/numerical models which only applicable in limited cases. In this presentation, I would like to present our efforts on overcoming the limitation of existing models and extending the scope of numerical approaches to describe experimentally observed microstructures, to predict new mesophases, to examine the suitability of different polymeric systems, as well as to provide the kinetic routes between various microphases in polymeric self-assembly. Here, we propose an efficient coarse-grained model that allows predicting the morphology of amphiphilic BCPs system over a wide range of chain architecture, concentrations, and solvent qualities. Model parameters are directed mapped to solvent quality and interfacial tensions of the systems through scaling analysis of single-chain size and molecular dynamic simulations.

Symposium : **PHYS3-3**

Recent Theoretical and Computer Simulation Studies of Macromolecules

Room 403 (Live Streaming) TUE 16:10

Chair: Sanghun Lee (Gachon University)

Computational study of self-assembled copper halide polymer nanowires: structure, properties, and applications

Kahyun Hur

Computational Science Research Center, Korea Institute of Science and Technology, Korea

Metal halide polymers are coordination polymers comprising of only metal and halogen atoms in the main backbone. The polymers have been extensively studied for decades, but their studies have been focused on synthesis and structure characterization, and materials properties and applications of metal halide polymers have been rarely investigated. We computationally studied recently reported copper halide polymers that can be readily synthesized in large quantities. The polymer self-assembles into a well-defined one-dimensional nanostructure and exhibits unique chemical and physical properties. Copper halide polymer nanowires have sub-nanometer pores that can absorb various metal ions and promote their catalytic activities as a single-atom support for electrochemical processes. Density functional theory calculations reveal the formation mechanism of copper halide polymer nanowires and the underlying physics of the unique electron transport properties of copper halide polymers. Molecular dynamics and grand canonical Monte Carlo simulations further demonstrate promising applications of metal halide polymers for water treatment, energy storage, and nanoreactors.

Symposium : **PHYS3-4**
Recent Theoretical and Computer Simulation Studies of Macromolecules
Room 403 (Live Streaming) TUE 16:30
Chair: Sanghun Lee (Gachon University)

Order-to-Disorder Transition of Block Copolymers in Thin Film: Self-consistent Field Theory and Langevin Field Theoretic Simulation

Jaeup Kim

Physics, Ulsan National Institute of Science and Technology, Korea

Nowadays block copolymer thin film became a standard material providing templates for nanoscience, but there still remain many fundamental questions regarding its phase transition and nanostructure alignment. In this study, we utilize three theoretical tools to investigate the formation of heterogeneous nanostructures and the effect of fluctuation.The first one is the discrete chain self-consistent field theory (DCSCFT) which provides the mean field theory of discrete bead model with the addition of finite-range interaction. We are especially interested in the effect of preferential and/or neutral interfaces on the shift of order-to-disorder transition (ODT) temperature, and the theoretical results are compared with experiments. The second one is the single chain in mean field (SCMF) simulation which allows polymer chains to make Monte Carlo moves under quasi-instantaneously updated self-consistent fields. By comparing free energy and natural period of the block copolymer phases, we systematically show that DCSCFT serves as an intermediate step between SCMF simulation and SCFT. In addition, we adopted angle dependent bond potential to simulate semiflexible polymers using bead-spring and freely-jointed chain models. It turns out that the lamellar domain has a tendency to align perpendicular to the surfaces when the chain stiffness is high. The last one is the Langevin field theoretical simulation (L-FTS). It is supposed to include the full compositional fluctuation of incompressible polymer melts, and its results are compared with the thin film ODT shifts predicted by the mean field theories.

Award Lecture in Division : **ANAL1-5**
Recent Advances in Mass Spectrometry based on Immunoaffinity
Room 301 (Live Streaming) TUE 14:30
Chair: Joohoon Kim (Kyung Hee University)

Metabolomics in human disease : advances and applications

Geum-Sook Hwang

Korea Basic Science Institute, Korea

The development of global metabolic profiling and the study of the metabolomics are particularly important in human disease where small molecules such as endogenous metabolites play fundamental signaling roles. Metabolomic approaches not only can help unravel the underlying molecular mechanism of disease but also identify the signature of pathway characteristic for specific disease that can be used for diagnosis, prognosis, and targeted therapy. Therefore, metabolomics-drived approaches have the potential to map biochemical changes in disease and provide an opportunity to unveil the metabolic pathways. This approach can also improve our understanding of the biological processes that are associated with a certain phenotype and also allow studying how the dysregulation of specific biological pathways is propagated across the biological system.

Analytical platforms, including NMR and Mass spectrometry, were used to generate a molecular fingerprint of biofluid or tissue samples, and then pattern recognition technique was applied to identify molecular signatures associated with the specific diseases or drug efficiency. Several metabolites that differentiate disease samples from the control were thoroughly characterized and the metabolic changes in human and animal model were investigated using analytical platforms. Spectral data were applied to targeted profiling and spectral binning method, and then multivariate statistical data analysis (MVDA) was used to examine in detail the modulation of small molecule candidate biomarkers. The metabolomic profiling process generates accurate metabolite concentration data, and provides data that can be used to help understand metabolic differences between healthy and disease or drug treated models. Such metabolic signatures could provide diagnostic markers for a disease state or biomarkers for drug response phenotypes, and mechanistic information on cellular perturbations and pathways associated with diseases.

Symposium : **ANAL1-2**

Recent Advances in Mass Spectrometry based on Immunoaffinity

Room 301 (Live Streaming) TUE 13:20

Chair: Wonryeon Cho (Wonkwang University)

Deciphering human B cell repertoire with next generation sequencing and mass spectrometry

Junho Chung

Department of Biochemistry and Molecular Biology, College of Medicine, Seoul National University, Korea

Facing infectious agents, human immune system develops adaptive immune responses in B cell and T cell repertoire. Only B cell receptor (BCR) undergoes somatichypermutation to achieve higher affinity toward antigens. B cells displaying BCR with the affinity above a threshold become plasma cells and actively secrete immunoglobulin reactive to the infectious agents to protect the host. Rapid development of NGS technology enabled us to decipher the peripheral B cell repertoire in a high throughput manner and with affordable cost. But it is still a hurdle to allocate antigen-reactive BCR sequence among the huge catalogue of BCR sequences. To tackle this problem, single cell sequencing after antigen-driven B cell sorting was introduced. Similarly, antibody display library and biopanning also can provide antigen-reactive BCR sequences. But all these technologies are nowhere near high throughput analysis. Only immune-affinity purification of antigen-reactive immunoglobulin and the determination of its peptide sequence using mass spectrometry can provide real high throughput data on the antigen-reactive BCRs. In this presentation, the current perspective on high throughput analysis of human B repertoire and its application to infectious disease will be discussed.

Symposium : **ANAL1-3**
Recent Advances in Mass Spectrometry based on Immunoaffinity
Room 301 (Live Streaming) TUE 13:40
Chair: Wonryeon Cho (Wonkwang University)

Clinical application of multiple reaction monitoring-mass spectrometry to HER2 measurements as a potential diagnostic tool for breast cancer therapy

Youngsoo Kim

Department of Biomedical Engineering, Seoul National University, Korea

Human epidermal growth factor receptor 2 (HER2) is often overexpressed in breast cancer and correlates with a worse prognosis. Thus, the accurate detection of HER2 is crucial for providing the appropriate measures for patients. However, the conventional techniques that are used to detect HER2 status are controversial. Specifically, fluorescence in situ hybridization (FISH), which is mandatory for arbitrating 2+ cases, is time-consuming and costly. To address this shortcoming, we established a multiple reaction monitoring-mass spectrometry (MRM-MS) assay that improves on existing methods for differentiating HER2 status.

We quantified HER2 expression levels in 210 breast cancer formalin-fixed paraffin-embedded (FFPE) tissue samples by MRM-MS assay. We aimed to improve the accuracy and precision of HER2 quantitation by simplifying the sample preparation through predicting the number of FFPE slides that was required to ensure an adequate amount of protein and using the levels of an epithelial cell-specific protein as a normalization factor when measuring HER2 levels.

To assess the correlation between MRM-MS and IHC/FISH data, HER2 expression levels from MRM-MS were divided by the expression levels of junctional adhesion molecule A (JAM1), an epithelial cell-specific protein, prior to statistical analysis. The normalized HER2 levels distinguished between HER2 2+/FISH-negative and 2+/FISH-positive groups (AUROC = 0.908), which cannot be differentiated by IHC. In addition, all HER2 status were discriminated by MRM-MS assay.

The novel MRM-MS assay yields more accurate HER2 expression levels relative to IHC, guiding clinicians toward the proper treatment for breast cancer patients, based on their HER2 expression.

Symposium : **ANAL1-4**
Recent Advances in Mass Spectrometry based on Immunoaffinity
Room 301 (Live Streaming) TUE 14:00
Chair: Wonryeon Cho (Wonkwang University)

Diagnosis of gastric cancer by targeted glycoproteomic approach using serum haptoglobin enriched by immunoaffinity chromatography

Hyun Joo An

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

Immunoaffinity chromatography is one of the most efficient techniques for enrichment and purification of a targeted protein (glycoprotein). Mass spectrometry is emerging as a powerful technique for analyzing the complexity and diversity of glycosylation due to its inherent sensitivity and accuracy. Recently, an analysis method combining an antibody-immobilized column and mass spectrometry has been widely used for disease diagnosis. Aberrant glycosylation of serum proteins has been linked to many human diseases including cancers. In particular, serum haptoglobin, a highly sialylated glycoprotein with four N-glycosylation sites, has gained considerable attention due to its potential as a signature molecule to display aberrant glycosylation in inflammatory disorders and various types of cancer. Here, we investigated in a multifaceted way to determine the relevance between serum haptoglobin glycosylation and gastric cancer. Haptoglobin was purified from the serum of gastric cancer patients and healthy control using an anti-haptoglobin antibody-conjugated column. For the detection of abnormal glycosylation, three different assay platforms were performed: glycan profiling, site-specific glycopeptide profiling, and intact protein profiling. These studies suggested that glycosylation variation of serum haptoglobin was associated with patients with gastric cancer and might be a promising marker for the cancer screening. Our platform, which provides biological information as well as high sensitivity and reproducibility, can be useful for gastric cancer biomarker discovery and diagnosis.

Symposium : **ANAL1-6**
Recent Advances in Mass Spectrometry based on Immunoaffinity
Room 301 (Live Streaming) TUE 15:00
Chair: Joohoon Kim (Kyung Hee University)

R&D on the intravenous diagnostic devices and their commercialization

Hakhyun Nam

R&D Center, i-SENS, Inc, Korea

Many analytical laboratories around the world publish their innovative detection methods on various biomarkers reporting substantially improved selectivity and sensitivity with higher accuracy, and often introduce new cartridge or sensor type tools that even non-specialist can easily handle to obtain sufficiently meaningful analytical results for diagnostic purpose. Some researchers patent their research outcomes hoping to attract possible business partners or even found their own company to commercialize them. However, very few of those efforts result in successful business due to the lack of understanding in market needs or failure in integrating necessary business resources. In this presentation, we will share our own experiences in the R&D's on various in vitro diagnostic (IVD) devices in our laboratory and commercialization efforts. Radically different idea and approaches are needed to mass produce and commercialize the simple biosensor strips and fluidic cartridges developed in the laboratory for the analysis of various metabolites and proteins. Also discussed are our past and current experiences in starting business with the products developed in the laboratory.

Symposium : **ANAL2-1**
Recent Advances in Environmental Mass Spectrometry
Room 301 (Live Streaming) TUE 15:40
Chair: Min-Sik Kim (DGIST)

Experimental study on the heterogeneous reaction of HCl with $MgCl_2$ and sea salt under humid conditions

Jong-Ho Park[*], **Andrey V. Ivanov**[1], **Mario J. Molina**[2]

Jeonbuk National University, Korea
[1]*Center of Biomedical Engineering, Sechenov University, Russia, Russia*
[2]*Department of Chemistry and Biochemistry, University of California-San Diego, USA, United States*

An experimental study on the heterogeneous reaction of HCl with sea salt and $MgCl_2$ under humid conditions was performed using a differential bead-filled flow tube system. The results indicate that the HCl uptake by the salt surfaces is enhanced in the presence of water vapor. Although the reactive sites are different for both the gaseous species, it is qualitatively the same as the OH uptake by sea salt under humid conditions, The humidity effects on $MgCl_2$ and sea salt for HCl uptake showed that the reaction site of a salt surface for HCl uptake is its absorbed water and that the overall rate is determined by the rate of water absorption. Based on the study of the dependence of γ_{HCl} on the initial HCl concentration, we estimate γ_{HCl} as 0.012 at 24% RH at a typical HCl concentration in the troposphere. The observation of the remarkable enhancement in the OH uptake by the HCl-treated salts agrees with the results of our previous studies, which suggested that water absorption on salts enhances γ_{OH} by lowering the surface pH. These results provide a basis for elucidating the contribution of the considered reactions to the heterogeneous chemistry of sea salt.

Symposium : **ANAL2-2**

Recent Advances in Environmental Mass Spectrometry

Room 301 (Live Streaming) TUE 16:00

Chair: Min-Sik Kim (DGIST)

Characterization of Chemicals Generated by Plastic Photolysis and Toxicity Evaluation

Sunghwan Kim

Department of Chemistry, Kyungpook National University, Korea

The impact of microplastics in the environment is a worldwide environmental concern. Particularly, various analytical methods have been developed and applied to characterize the types of microplastics and particle sizes in the environment. Kyungpook National University's Environmental & Energy Mass Spectrometry Lab (EEMSLab) conducts research in three main directions. The first is the development and application of spectroscopic methods to measure the shape of nano-sized particles. The second is to develop and apply a mass spectrometry based method for qualitative and quantitative determination of compounds produced by plastic degradation in the environment. Finally, toxicity test is performed to measure the environmental influence of photo degraded plastic materials. In this presentation, the results obtained by EEMSLab up to date will presented.

Symposium : **ANAL2-3**
Recent Advances in Environmental Mass Spectrometry
Room 301 (Live Streaming) TUE 16:20
Chair: Min-Sik Kim (DGIST)

Application of Suspect/non-target screening to identify transformation products of pesticides formed in a natural wetland

Junho Jeon

Environmental analytical chemistry, Changwon National University, Korea

Natural wetlands have been recognized as a bio-reactor for degradation and elimination of environmental pollutants (e.g., pesticides). The aim of this study was to identify degradation (or transformation) products of pesticides in the wetland using LC-HRMS based suspect/non-target screening and evaluate the elimination ability of wetland. We used QExactiv Orbitrap with a two-step analysis approach (i.e., 1st analysis for target measurement along with suspect and non-target screening (SNTS) and 2nd analysis for complimentary suspect screening) to identify and quantify the transformation products (TPs) of the identified major pesticides. Quantitative analysis of 30 targets, mainly including pesticides, showed that fungicides were the major contaminants detected in the wetland. Orysastrobin occurred at the highest mean concentration (>700 ng/L), followed by two other fungicides, carbendazim and tricyclazole. The first analysis (SNTS) tentatively identified 39 TPs (30 by suspect, 9 by non-target screening) of 14 parent pesticides. Additionally, the second analysis (complimentary suspect screening) identified 9 more TPs. Among the 48 total TPs identified, 7 were confirmed with reference standards. The identification of the remaining TPs had a high confidence level (e.g., level 2 or 3). Regarding transport though the wetland, most TPs showed greater peak area ratios (i.e., the relative portion of chromatographic area of the TPs to the parent compound) at the outlet point of the wetland compared to the inlet point. The estimates for biodegradability, hydrophobicity, and toxicity by an in-silico quantitative structure-activity relationship (QSAR) model indicated a lower half-life, lower logDOW, and greater effect concentration for most TPs compared to the parent compounds. Based on these results, we conclude that natural wetlands play a role as an eco-friendly reactor for degrading pesticide to form numerous TPs that are lower risk than the parent compounds.

Symposium : **ANAL2-4**
Recent Advances in Environmental Mass Spectrometry
Room 301 (Live Streaming) TUE 16:40
Chair: Min-Sik Kim (DGIST)

Target and non-target analysis of organic micropollutants in surface water using LC-orbitrap MS

Injung Lee

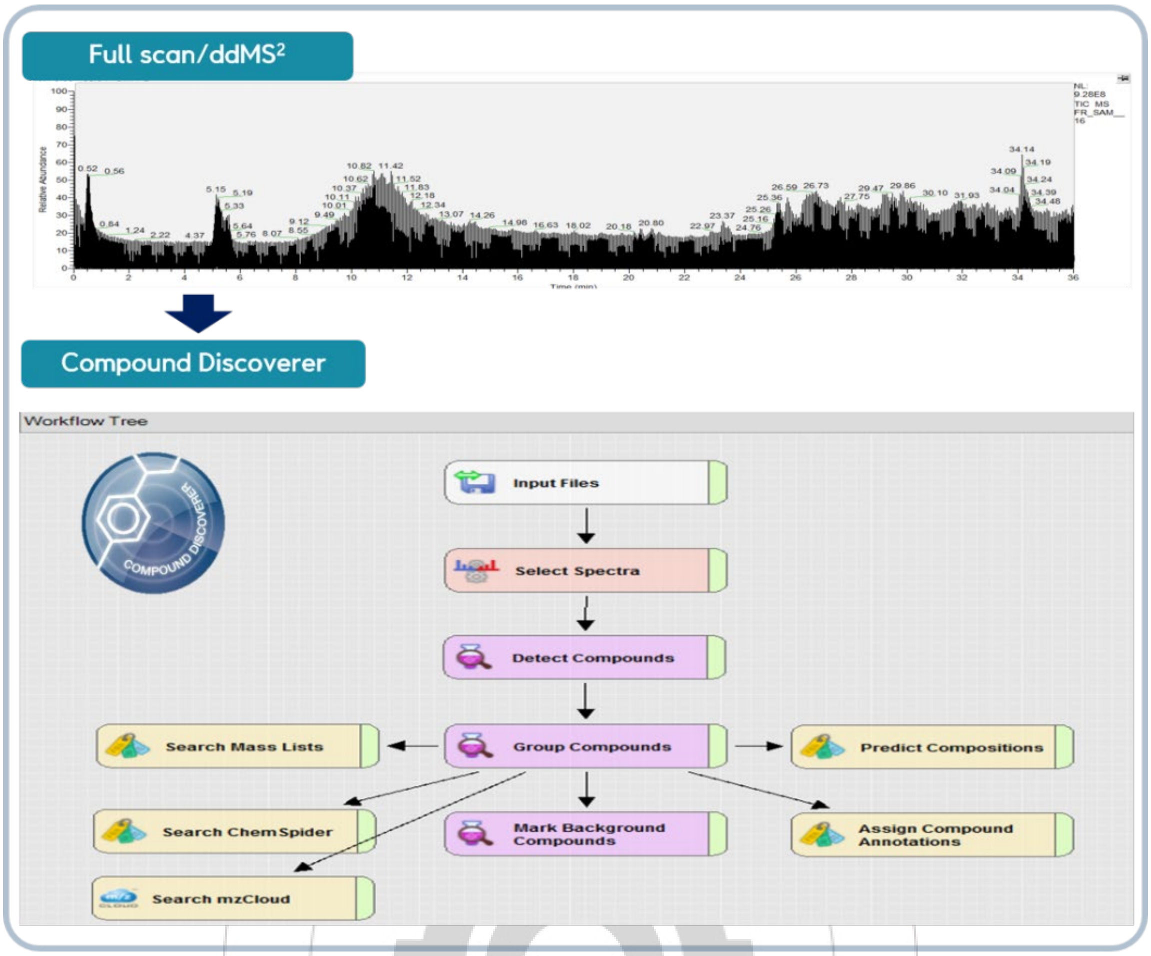
Water Environment Research Department, National Institute of Environmental Research, Korea

Emerging contaminants are a diverse group of non-regulated micropollutants such as pharmaceuticals and personal care products (PPCPs), pesticides, endocrine disrupting compounds (EDCs), etc. It has been detected at trace levels in various environmental samples such as surface water, soil, sediment, and aquatic biota. The occurrence of micropollutants in environmental samples can negatively impact the health of the ecosystem and humans. The objective of this study is to determine the target micropollutants and to identify unknown micropollutants in surface water.

We categorized 94 organic micropollutants containing PPCPs, pesticides, and industrial chemicals for target analysis. An liquid chromatography-tandem mass spectrometric (LC-MS-MS) method was developed for rapid simultaneous determining of 94 organic micropollutants. The method was validated in terms of linearity, limit of detection (LOD), limit of quantitation (LOQ), accuracy, and precision. The adequate values were obtained. The concentrations of 94 compounds were determined in surface water and 72 compounds were detected at trace levels, ranging from ng/L to μg/L.

Also, non-target screening method was established using LC-orbitrap MS and Compound Discoverer software provided by Thermo Scientific to identify unknown micropollutants in surface water. The detected compounds were estimated by matching MS spectrum (full scan/ddMS2) and with chemical structure or MS database such as ChemSpider, mzCloud, and mzVault. We finally identified 14 compounds in surface water samples by applying peak area of 1.0E6 or more, and matching with in silico fragment ion search. It is needed to confirm the compounds by qualitative and quantitative analysis using reference standard materials.

It will be used to list the priority compounds for the management of hazardous chemicals by target and non-target analysis.


Full scan/ddMS^2
Relative Abundance
100
90
80
70
60
50
40
30
20
10
0
0.52 0.56
0.84
1.24
2.22
4.37
5.15 5.19
5.33
5.64
5.76
8.07
9.12
8.55
9.49
10.01
10.11
10.37
10.62
10.82 11.42
11.52
11.83
12.18
12.34
13.07 14.26
14.98
16.63
18.02
20.18
20.80
22.97
23.37
24.76
25.16
25.26
25.36
26.59 26.73
27.75
29.47 29.86
30.10
31.93
34.04
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34.48
NL:
9.28E8
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Compound Discoverer
Workflow Tree
COMPOUND DISCOVERER
Input Files
Select Spectra
Detect Compounds
Search Mass Lists
Group Compounds
Predict Compositions
Search ChemSpider
Mark Background Compounds
Assign Compound Annotations
Search mzCloud

Award Lecture in Division : **LIFE1-1**
Recent Trends in Chemical Biology Research
Room 305 (Live Streaming) TUE 10:00
Chair: Eun Gyeong Yang (KIST)

Engineering artificial protein assemblies to study and use biomolecular assemblages

Yongwon Jung

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

Biological systems are highly complicated but at the same time remarkably precise and dynamic. These systems are built through well-organized self- (or assisted-) assembly processes of various biomolecules such as DNA/RNA, proteins, and lipids. In particular, proteins are major building blocks for these precisely organized assemblages by virtue of their abundant structures and functions. Many artificial protein assemblies have been investigated with the aim of understanding natural assembly processes as well as devising novel biomolecular architectures with new structures and functions. A major research goal in our group is to create precise nano-assemblies of functional proteins with both defined structures and a controlled number of protein building blocks. With these protein assemblies, we aim to conduct or control highly precise but dynamic behaviors of supramolecular bio-assemblages. Here, I will introduce several our newly developed artificial protein assemblies with defined valency and structures. Examples of a few bio-analytical and medical tools that utilize these protein assemblies will be presented. In addition, I will discuss a recently emerging concept of biomolecular liquid-liquid phase separation, which is also heavily governed by protein assembly processes.

Symposium : **LIFE1-2**
Recent Trends in Chemical Biology Research
Room 305 (Live Streaming) TUE 11:00
Chair: Jiwon Seo (GIST)

Siderophore-based drug delivery as an effective approach to overcome the antibiotic resistance of the human pathogen, *Acinetobacter baumannii*

Hak Joong Kim

Department of Chemistry, Korea University, Korea

The rapid emergence of drug resistant pathogens such as *Acinetobacter baumannii* has been of serious threat to human welfare, but development of effective antibacterial therapies to combat against this problem has been procrastinated. Acknowledgement of such grave status calls for exploitation of alternative therapeutic modalities, conceptually unbound by the conventional antibacterial regimen. Our laboratory has been interested in experimenting various ideas on development of new siderophore-based antibacterial modalities. Siderophores are small-molecule metal chelators that are key molecules for bacterial iron acquisition. Since the siderophore-based metabolism is one of the key virulence factors essential for the survival of pathogens in the infection site, perturbation of this mechanism has been considered as an attractive novel target for antimicrobial discovery. In this presentation, a short summary of our recent studies on the siderophore metabolism in *A. baumannii* as well as some of the progresses on the siderophore-based antibacterial strategies will be discussed

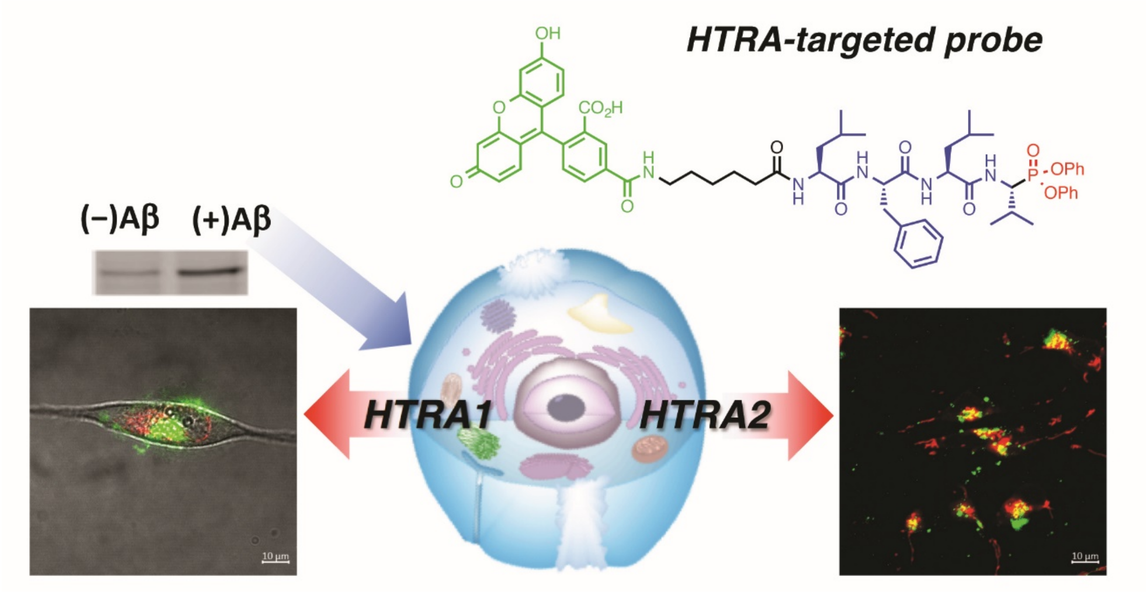
Symposium : **LIFE1-3**
Recent Trends in Chemical Biology Research
Room 305 (Live Streaming) TUE 11:20
Chair: Jiwon Seo (GIST)

Reactivity-based fluorescent probes for studying enzyme functions in living systems

Jiyoun Lee

Global Medical Science, Sungshin Women's University, Korea

All biological components in living organisms including genes, molecules and cells, communicate and cooperate via an array of intricate and complex pathways. Recent advances in molecular biology and genetics have aided scientists in elucidating the complex pathways and processes in biological systems. While some of these pathways have already been discovered, many more remain to be explored. Chemical biology provides a unique approach to study biological systems by using synthetic small molecules. Unlike common biological methods involving genetic engineering and immunochemistry, small molecule chemical tools can be delivered easily and modified readily with high specificity. Our research goal is to develop small molecule chemical tools to study enzyme functions and expand these tools to generate diagnostic imaging and therapeutic agents to treat various diseases. In this talk, I will discuss our ongoing research efforts focusing on the reactivity-based fluorescent probes to detect intracellular ions and proteases. We utilize intracellular chemical reactions to generate specific fluorescent signals in response to the presence of various analytes, and eventually to monitor functional activity of cysteine and serine proteases in cell-based neurodegenerative disease models. In recognition of the emerging importance of mitochondrial function in neurodegenerative diseases, we also developed a mitochondria-targeting molecular transporter and used it to deliver fluorescent probes to detect mitochondrial enzyme activity.


HTRA-targeted probe
OH
O
CO$_2$H
O
H
N
O
N
H
O
H
N
O
N
H
O
H
N
O
P
OPh
OPh
(−)Aβ
(+)Aβ
HTRA1
HTRA2
10 μm
10 μm

Symposium : **LIFE1-4**
Recent Trends in Chemical Biology Research
Room 305 (Live Streaming) TUE 11:40
Chair: Jiwon Seo (GIST)

Photo-activation approach to spatio-temporal mapping for biomolecule interactions in complex biological environment

Jun-Seok Lee

Molecular Recognition Research Center, Korea Institute of Science and Technology, Korea

Protein-protein interactions (PPIs) trigger a wide range of biological signaling pathways that are crucial for biomedical research and drug discovery. Various techniques have been used to study specific proteins, including affinity chromatography, activity-based probes, affinity-based probes and photo-affinity labeling (PAL). Recently, we report the first rational design of a photo-crosslinking BODIPY fluorophore (pcBD) and its biological application for biomolecule labeling. As a photosensitizing functional motif, an aryl ketone group was incorporated into the BODIPY fluorophore, and a series of proteins were labeled by pcBD compounds upon UV irradiation. In order to investigate protein–protein interactions in a protein mixture, amino-functionalized pcBD was prepared and covalently attached to a ubiquitin ligase binding peptide. Upon UV irradiation, we could successfully visualize the substrates in the total lysate. These results provided a proof of concept for spatially controllable tagging via photo-activation of the pcBD scaffold and demonstrated its potential usage for in situ labeling applications. In addition to photo-affinity fluorophore scaffold, we also examined series of photo activatable functional groups, including tetrazole. Photolysis of tetrazoles to nitrile imines are extremely rapid and efficient process and the light-induced tetrazole-alkene 1,3-dipolar cycloaddition (also known as tetrazole photoclick chemistry) was first reported as a bioorthogonal reaction in 2008 by Lin’s group. We explored the alternative use of the tetrazole photoclick reaction inspired by the high electrophilicity of nitrile imine species and revealed nucleophilic side chain of protein could generate chemical crosslinking. In this presentation, we will discuss photo-activatable crosslinking approach to investigate cellular organelle proteomics.

Symposium : **LIFE2-1**
Recent Progress in Life Chemistry
Room 305 (Live Streaming) TUE 13:00
Chair: Seokhee Kim (Seoul National University)

Single-molecule Force Spectroscopy Unfolds Membrane Protein Folding Mystery

Duyoung Min

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

Membrane proteins carry out many vital tasks across the cell membrane and they are the largest class of drug targets. One of great challenges in membrane protein chemistry is to learn how they fold into their structures (the membrane protein folding problem). Protein misfolding is the cause of many genetic diseases, so fundamental folding studies will have broad medical impact. However, most of the effort to understand the folding has bypassed membrane proteins because of demanding technical challenges. By developing and using single-molecule force spectroscopy, I have been seeking to understand how membrane proteins (un)fold and their potential biological implications. In this talk, I will present a unique single-molecule method that I have developed to study membrane protein folding problem, one application of the technique to an extremely complex ClC chloride transporter, a touch of delicate lipid effects on the folding, and a recent technical advance in the actual folding measurement. Single-molecule methods are particularly useful in membrane protein studies as the hydrophobic aggregation problem can be intrinsically obviated. Understanding (mis)folding is a key to designing therapeutic strategies to combat misfolding diseases, so we can ultimately contribute to medicine as well as fundamental folding chemistry.

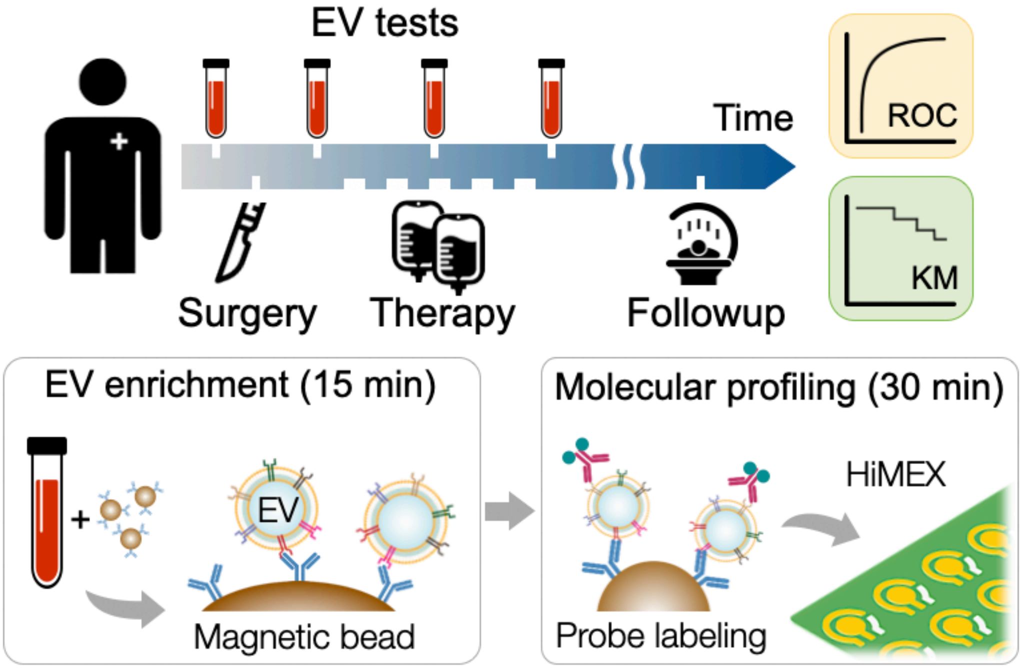
Symposium : **LIFE2-2**
Recent Progress in Life Chemistry
Room 305 (Live Streaming) TUE 13:25
Chair: Seokhee Kim (Seoul National University)

Immunomagnetic Electrochemical Sensor for Extracellular Vesicle Analysis and Disease Diagnosis

Jongmin Park

department of Chemistry, Kangwon National University, Korea

Extracellular vesicles, including exosomes, are nanoscale membrane particles that carry molecular information on parental cells. They are being pursued as biomarkers of various diseases, especially cancer that are difficult to detect or serially follow. To solve this issue, we developed a compact sensor technology for rapid, on-site exosome screening. The sensor is based on an integrated magneto−electrochemical assay: exosomes are immunomagnetically captured from patient samples and profiled through electrochemical reaction. By combining magnetic enrichment and enzymatic amplification, the approach enables (i) highly sensitive, cell-specific exosome detection and (ii) sensor miniaturization and scale-up for high-throughput measurements. We demonstrated this system to screen extracellular vesicles in human body fluids such as plasma or urine samples from patients with ovarian cancer, kidney transplant rejection and colorectal cancer patients. The sensor allowed for the simultaneous profiling of multiple protein markers within an hour, outperforming conventional methods in assay sensitivity and speed.


EV tests
Time
ROC
KM
Surgery
Therapy
Followup
EV enrichment (15 min)
EV
Magnetic bead
Molecular profiling (30 min)
HiMEX
Probe labeling

Symposium : **LIFE2-3**
Recent Progress in Life Chemistry
Room 305 (Live Streaming) TUE 13:50
Chair: Seokhee Kim (Seoul National University)

Multiplexed, scalable gene editing platform for modeling cancer and identifying effective cancer therapy

Tackhoon Kim

Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea

Cancer is rarely a monogenic disease. Nor is cancer therapy feasible with targeting single oncogene. There is an urgent need for platforms that enable multiplexed gene editing to account for complex genetic alterations in cancer, and also to identify drug targets which synergize when targeted together. Here I discuss two breakthroughs that enable CRISPR-Cas9 based genetic engineering and screening platforms. First part of the talk will introduce combinatorial CRISPR screens that identified novel combination of tyrosine kinase inhibitors that synergize for treating triple negative breast cancer (TNBC). FYN tyrosine kinase was identified as an adjuvant target whose inhibition can synergistically treat TNBC both in vitro and in vivo with wide range of tyrosine kinase inhibitors such as IGF1R, EGFR and ABL inhibitors. The second part of the talk will introduce novel gene circuit that enables multiplexed, sequential gene expression platform that can be used as the next generation tumorigenesis model by the accumulation of mutations over time. This gene circuit was successfully implemented to sequentially introduce indel mutation at key tumor suppressor genes at any desired time point. These highly innovative genetic engineering and screening platforms will potentially revolutionize current practices in cancer research and cancer therapeutics.

Symposium : **LIFE2-4**
Recent Progress in Life Chemistry
Room 305 (Live Streaming) TUE 14:15
Chair: Seokhee Kim (Seoul National University)

Quantitative super-resolution microscopy unveils molecular mechanisms of platelet activation and release

Doory Kim

Department of Chemistry, Hanyang University, Korea

Platelets are anucleate cytoplasmic fragments generated from megakaryocytes and have major roles in hemostasis. Recent emerging evidence demonstrates that platelets are equipped with elaborate intracellular machinery, and their organization is far more complex than previously regarded. However, their ultrastructural organization in platelets in the different stages of activation or maturation process remains unclear due to the difficulty in determining and quantifying the ultrastructure of platelets by diffraction-limited conventional light microscopy. To overcome this limit, we used stochastic optical reconstruction microscopy to resolve the native ultrastructure and their interaction of different organelles in platelets. The recent development of super-resolution fluorescence microscopy allows the location of molecules to be determined with nanometer-scale spatial resolution. Moreover, correlative super-resolution microscopy, the integration of the high spatial resolution of super-resolution fluorescence microscopy with other imaging platforms, offers intriguing opportunities to probe multiple aspects of a given system. By using these approaches, we quantitatively characterized nanoscale localization changes of organelles, including cytoskeletal elements, mitochondria, endoplasmic reticulum, and granules in a platelet during its activation and release process. Our results highlight how different organelles are spatiotemporally organized in the different intermediate stages during the platelet activation and release process. We anticipate that these techniques would open up a new way to study ultra-structures of organelles in platelets, and will shed light on the fundamental molecular mechanisms of platelet structure and function.

Symposium : **LIFE2-5**
Recent Progress in Life Chemistry
Room 305 (Live Streaming) TUE 14:40
Chair: Seokhee Kim (Seoul National University)

Investigation of the mechanism of the SpnF-catalyzed [4+2]-cycloaddition reaction in the biosynthesis of spinosyn A

Byungsun Jeon

Center for Neuro-Medicine, Korea Institute of Science and Technology, Korea

Diels-Alder reaction is one of the most prominent name reaction to chemically synthesize a six-membered cyclohexene. While it has long been proposed that the cyclohexene moiety found in many secondary metabolites is also introduced via enzyme-catalyzed Diels-Alder reaction. The SpnF involved in the biosynthesis of insecticide spinosyn A in the actinomycete bacteria Saccharopolyspora spinosa is the first enzyme whose catalysis of an intramolecular [4+2] cycloaddition has been experimentally verified as its only known function. Since its discovery, a number of additional [4+2]-cyclases have been reported as potential Diels-Alderases; however, whether their catalytic cycles involve a concerted or stepwise cyclization mechanism has not been addressed experimentally. Here, we report the first direct experimental interrogation of the reaction coordinate for the [4+2]-carbocyclase. SpnF via the measurement of α-secondary deuterium kinetic isotope effects (KIEs) at all sites of sp2→sp3 rehybridization for both the nonenzymatic and enzymatic cyclization of the SpnF substrate. The measured KIEs for the nonenzymatic reaction are consistent with previous computational results implicating an intermediary state between formation of the first and second carbon-carbon bonds. The KIEs measured for the enzymatic reaction suggest a similar mechanism of cyclization within the enzyme active site; however, there is evidence that conformational restriction of the substrate may play a role in catalysis.

Award Lecture in Division : **ORGN1-1**
Current Trends in Organic Chemistry I: Medicinal Chemistry & Chemical Biology
Room 306 (Live Streaming) TUE 10:50
Chair: Seunghoon Shin (Hanyang University)

Exploring Novel Ligand Designs for Catalytic Organic Synthesis

Sukwon Hong

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

Research in the Hong group focuses on the development of transition metal catalysts for organic synthesis. In particular, research efforts have been directed toward the development of cooperative asymmetric catalysts and N-heterocyclic carbene (NHC) ligands, and their applications in asymmetric organic synthesis, sustainable chemistry, and organic materials science. In this 2020 Sehi Jang award lecture, recent results will be discussed including cation-binding salen nickel catalysts for enantioselective alkynylations, pyridine-dihydroisoquinoline ligands for asymmetric conjugate arylations, NHC-palladium catalysts for olefin polymerization, and NHC-ruthenium catalysts for the olefin metathesis with ethylene.

Symposium : **ORGN1-2**

Current Trends in Organic Chemistry I: Medicinal Chemistry & Chemical Biology

Room 306 (Live Streaming) TUE 11:15

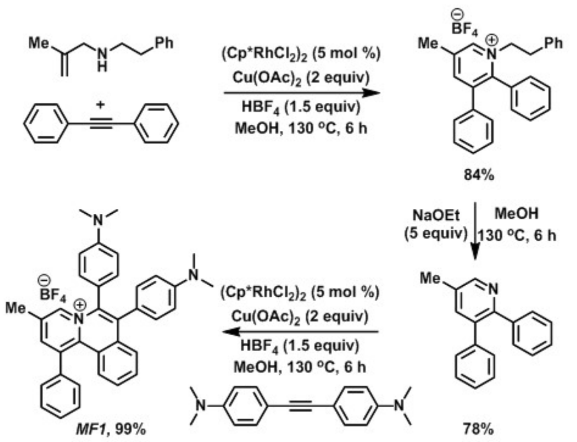
Chair: Soo Hyuk Choi (Yonsei University)

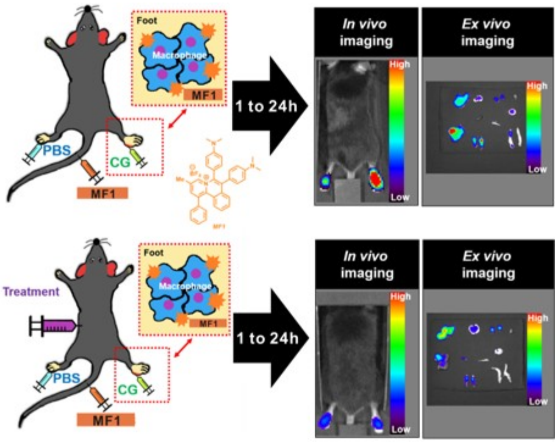
Synthesis of Rh(III)-catalyzed N-heterocyclic compounds and their application to inflammation imaging agent

Sangbong Lee, Ye Ri Han[1], Chul-Ho Jun[2], Sung Jin Cho[1,*], Dong-Su Kim[3,*]

Nano-Bio materials lab, Korea Institute of Medical Microrobotics (KIMIRo), Korea
[1]*Daegu Gyeongbuk Medical Innovation Foundation, Korea*
[2]*Department of Chemistry, Yonsei University, Korea*
[3]*Therapeutics and Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

The N-heterocyclic compounds represent ubiquitous structural motifs such as biologically active compounds and functional materials. With the many studies of C-H bond activation reactions, various method employing Rh(III)-catalysis have been developed for the synthesis of N-heterocylic compounds. Recently, we developed new synthetic methods for the synthesis of pyridinium and benzoquinolinium salts using Rh(III)/Cu(II) complex. Interestingly, it has been found that these heterocyclic compounds are fluorescent materials and their emission wavelength can be adjusted by employing different internal alkynes. Based on these results, we have attempted the application of fluorescent materials to in vivo model diagnostic bioimaging. For successful application of fluorescent materials as imaging agent, several in vitro and in vivo experiments have been performed. As a result, we found that benzoquinolizinium salt can act as an in vivo imaging agent for detection of inflammatory lesions. This result can be applied to the diagnosis of disease.


Me
N
H
Ph
+
(Cp*RhCl$_2$)$_2$ (5 mol %)
Cu(OAc)$_2$ (2 equiv)
HBF$_4$ (1.5 equiv)
MeOH, 130 °C, 6 h
BF$_4$
Me
N
Ph
84%
NaOEt
(5 equiv)
MeOH
130 °C, 6 h
Me
N
78%
(Cp*RhCl$_2$)$_2$ (5 mol %)
Cu(OAc)$_2$ (2 equiv)
HBF$_4$ (1.5 equiv)
MeOH, 130 °C, 6 h
N
N
BF$_4$
Me
N
N
MF1, 99%


Foot
Macrophage
MF1
PBS
CG
MF1
1 to 24h
In vivo imaging
Ex vivo imaging
High
Low
Treatment
Foot
Macrophage
MF1
PBS
CG
MF1
1 to 24h
In vivo imaging
Ex vivo imaging
High
Low

Symposium : **ORGN1-3**

Current Trends in Organic Chemistry I: Medicinal Chemistry & Chemical Biology

Room 306 (Live Streaming) TUE 11:35

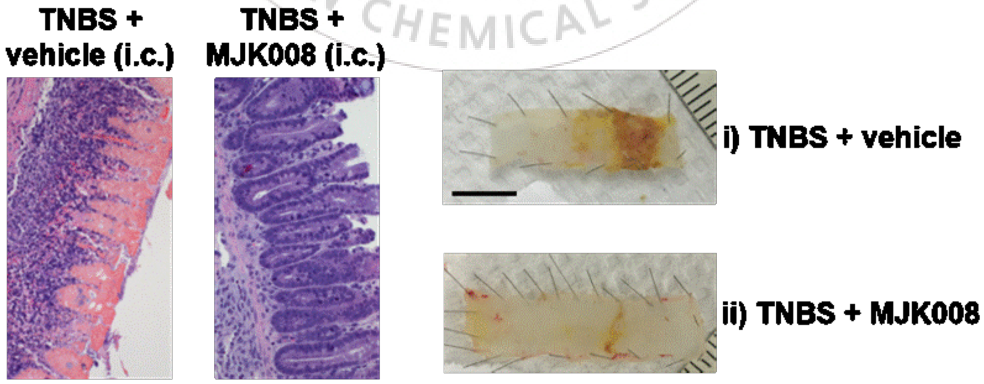
Chair: Soo Hyuk Choi (Yonsei University)

Development of HDAC Inhibitors for Treatment of Inflammatory Bowel Disease

Jonghoon Kim

Department of Chemistry, Soongsil University, Korea

Epigenetic alterations have been involved in the pathogenesis of cancer and auto-immune diseases, including Crohn's Disease, Ulcerative Colitis, Lupus and Rheumatoid Arthritis. Histone deacetylases (HDACs), a key component of the epigenetic machinery, are enzymes that catalyze the removal of acetyl functional groups from the lysine residues of both histone and non-histone proteins. There are 18 isotypes of HDACs with different functions in different disease settings. Therefore, the development of HDAC inhibitor with isoform-selectivity may provide important new tools for treatment of auto-immune diseases. To date, MC-1568 (MJK001) analogues were designed and synthesized to target HDAC9 for treatment of inflammatory bowel disease (IBD), one of the auto-immune diseases



Daily intracolonic injections of MJK008 substantially decrease the severity of experimental colitis *in vivo*. Representative histological sections (10X) and colonic ulcerations from mice with TNBS colitis following daily intracolonic injections with vehicle or MJK008.

Symposium : **ORGN1-4**

Current Trends in Organic Chemistry I: Medicinal Chemistry & Chemical Biology

Room 306 (Live Streaming) TUE 11:55

Chair: Soo Hyuk Choi (Yonsei University)

Design, Synthesis, and Anti-RNA Virus Activity of 6′-Fluorinated-Aristeromycin Analogues

Gyudong Kim, Lak Shin Jeong[1,*]

College of Pharmacy, Chonnam National University, Korea

[1]*Department of Pharmacy, Seoul National University, Korea*

(−)-Aristeromycin, isolated from Streptomyces citricolor, is a representative carbocyclic nucleoside that exists in nature. This compound is a potent inhibitor of S-adenosylhomocysteine (AdoHcy) hydrolase and shows potent antiviral activities against several RNA and DNA viruses. Based on this natural product, (−)-6′-β-fluoro-aristeromycin has been synthesized via stereoselective electrophilic fluorination followed by a purine base build-up approach. And the 6′-fluorinated aristeromycin analogues were designed as dual-target antiviral compounds aimed at inhibiting both the viral RNA-dependent RNA polymerase (RdRp) and the host cell S-adenosyl-L-homocysteine (SAH) hydrolase, which would indirectly target capping of viral RNA. The introduction of a fluorine at the 6′-position enhanced the inhibition of SAH hydrolase and the activity against RNA viruses.References1. Yoon, J-S.†; Kim, G.†; Jarhad, D. B.; Kim, H-R.; Shin, Y-S.; Qu, S.; Sahu, P. K.; Kim, H. O.; Lee, H. W.; Wang, S. B.; Kong, Y. J.; Chang, T-S.; Ogando, N. S.; Kovacikova, K.; Snijder, E. J.; Posthuma, C. C.; van Hemert, M. J.; Jeong, L. S. “Design, Synthesis, and Anti-RNA Virus Activity of 6′-Fluorinated-Aristeromycin Analogues” J. Med. Chem. 2019, 62, 6346-6362. (†1st co-author)2. Kim, G.; Yoon, J.-S.; Jarhad, D. B.; Shin, Y. S.; Majik, M. S.; Mulammutti, V. A.; Hou, X.; Qu, S.; Park, J.; Baik, M.-H.; Jeong, L. S. “Asymmetric Synthesis of (-)-6'-b-Fluoro-aristeromycin via Stereoselective Electrophilic Fluorination” Org. Lett. 2017, 19, 5732-5735.

Symposium : **ORGN1-5**
Current Trends in Organic Chemistry I: Medicinal Chemistry & Chemical Biology
Room 306 (Live Streaming) TUE 12:15
Chair: Soo Hyuk Choi (Yonsei University)

Synthesis of Azacycles & Development of Novel Fluorinated Pyrazolopyrimidine Derivatives

Hee-Kwon Kim

Department of Nuclear Medicine, Jeonbuk National University, Korea

Part 1. *N*-Substituted azacycles is one of the important units in medicinal chemistry and organic chemistry. Particularly, *N*-substituted azacycles are currently found in many bioactive materials such as drugs as well as hormones and vitamins. Therefore several synthetic protocols have been developed, and most of preparations of azacyles were achieved by the employment of various metal reagents. Thus, synthetic method without metal is the one of the meaningful challenges to prepare azacycle. Herein, a novel efficient metal-free protocol for the synthesis of *N*-aryl substituted azacycles has been described. In this study, various arylamines were successfully reacted with cyclic ethers in the presence of phosphorus (V) oxychloride and bases to produced five- and six-membered azacycles with high yield. Part 2. It was reported that translocator protein (TSPO), which is mitochondrial 18k Da translocator protein, plays crucial roles in neuroinflammation and neuronal damage, and pyrazolopyrimidine structure showed high and selective affinity to TSPO. In this study, a series of fluorinated pyrazolopyrimidine derivatives was synthesized via cyclization and fluorination. And newly prepared compounds was successfully employed to detect neuroinflammation in brain

Symposium : **ORGN2-1**
Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis
Room 306 (Live Streaming) TUE 13:30
Chair: Cheol-Hong Cheon (Korea University)

An Enantioselective N-Heterocyclic Carbene-Catalyzed Decarboxylative [4+2] Cycloaddition

Ansoo Lee

Center for Neuro-Medicine, Korea Institute of Science and Technology, Korea

Chemical reaction is a crucial component of our everyday lives. The most powerful and efficient chemical reactions commonly use catalysis to control reactivity and selectivity. Thus, the discovery of new catalysis with broad utility beyond established reactivity will give a great impact on academic and industrial organic synthesis.Herein, I will discuss our finding on a new N-heterocyclic carbene (NHC) organocatalysis. We recently discovered a direct decarboxylative strategy for the generation of aza-o-quinone methides (aza-o-QMs) by NHC catalysis. The NHC-bound aza-o-QM intermediate reacts with activated ketones through a formal [4+2] manifold to access highly enantioenriched products. The effect of using electron-rich NHCs on the reactivity and enantioselectivity will be discussed. Furthermore, an interesting stereoretentive aza-Petasis-Ferrier rearrangement will be described.

Symposium : **ORGN2-2**
Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis
Room 306 (Live Streaming) TUE 13:50
Chair: Cheol-Hong Cheon (Korea University)

Visible-Light Induced Cysteine-Specific Bioconjugation

Jaebong Jang

College of Pharmacy, Korea University, Korea

The chemistry-based modification of biomolecules has been intensively studied for the advancement of chemical biology, molecular biology, and drug development. One of the representative applications of bioconjugation is the successful development of antibody-drug conjugates that promotes studies on the development of reliable methods amenable to site- and chemo-selective protein modification. Recently, visible-light photocatalysis has emerged as a powerful tool in bioconjugation for the selective modification of biomolecules under mild reaction conditions. However, the number of photochemical transformations that allow successful protein bioconjugation is still limited due to the need for stringent reaction conditions. Herein, we report that a water-compatible fluorescent photosensitizer QPEG can be used for visible-light-induced cysteine-specific bioconjugation, which can directly install QPEG itself onto proteins by exploiting its intrinsic photosensitizing ability to activate the S–H bond of cysteine. In addition, the slightly modified QCAT enables the effective photocatalytic and cysteine-specific conjugation of biologically relevant chemicals. The superior reactivity and cysteine selectivity of this methodology was further corroborated by traceless bioconjugation with a series of complex peptides and proteins under biocompatible conditions.

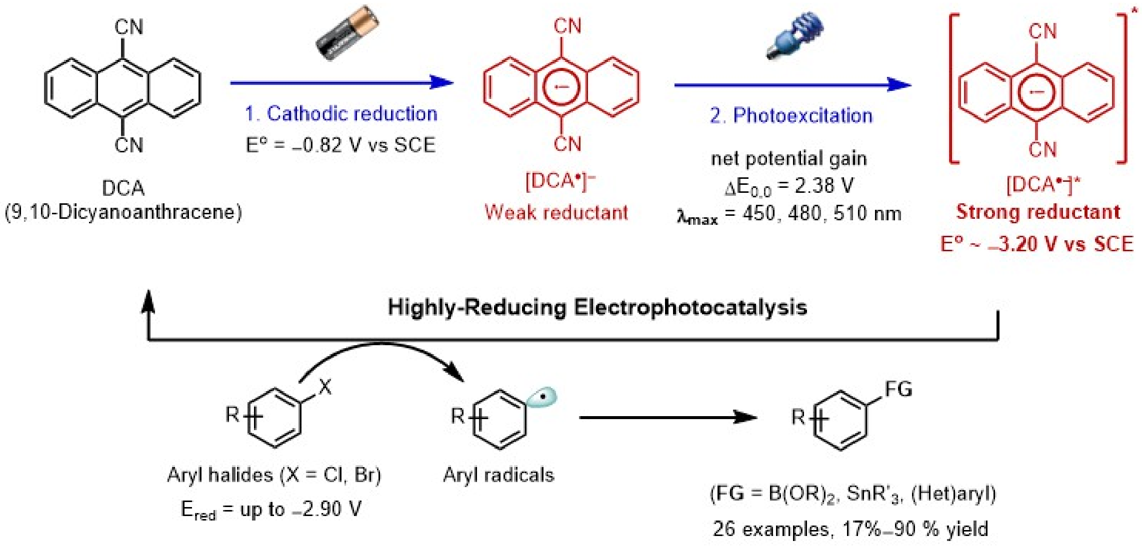
Symposium : **ORGN2-3**
Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis
Room 306 (Live Streaming) TUE 14:10
Chair: Cheol-Hong Cheon (Korea University)

Modern Electrocatalysis for Sustainable Organic Synthesis: Generation of Exotic Radical Species by Unconventional Means of Single-Electron Transfer Reaction

Hyunwoo Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Due to the unique reactivity of open-shell intermediates, the development of catalytic transformations driven bysingle-electron transfer (SET) has been an area of intense research in organic chemistry. In particular, the employment of unconventional means of activation, including photoredox catalysis and electrocatalysis, has provided unique entry to single-electron reactivities and led to new solutions to challenging synthetic problems that are not readily addressed using existing tools. In the realm of redox organic reactions, both photoredox catalysis and electrochemistry have been successfully applied to a diverse suite of transformations. However, reductive transformations remain an underdeveloped area for both of these reaction strategies. In principle, electrochemistry can grant access to extreme reducing potentials, and significant contributions in this regard have recently been made. Nevertheless, the constant application of such highly biased potentials can lead to uncontrolled reactions due to accumulation of reactive intermediates near the electrode surface as well as compromised chemoselectivity in complex reaction systems. Thus, the development of catalytic strategies that are both highly reducing and also chemoselective remains a major challenge. In this symposium, we present a new electrophotocatalytic strategy enables extremely reducing intermediates via tandem cathodic reduction and photoexcitation under mild reaction conditions.


CN
CN
DCA
(9,10-Dicyanoanthracene)
1. Cathodic reduction
E° = −0.82 V vs SCE
[DCA•]⁻
Weak reductant
2. Photoexcitation
net potential gain
ΔE0,0 = 2.38 V
λmax = 450, 480, 510 nm
[DCA•⁻]*
Strong reductant
E° ~ −3.20 V vs SCE
Highly-Reducing Electrophotocatalysis
X
R
Aryl halides (X = Cl, Br)
Ered = up to −2.90 V
Aryl radicals
FG
(FG = B(OR)2, SnR'3, (Het)aryl)
26 examples, 17%−90 % yield

Symposium : **ORGN2-4**

Current Trends in Organic Chemistry II: Synthetic Methodology and Catalysis

Room 306 (Live Streaming) TUE 14:30

Chair: Cheol-Hong Cheon (Korea University)

Origins of Selectivity and Reactivity in Isothiourea-Catalyzed Asymmetric Transformations: Traditional and New Approaches to Generation of Hypotheses

Paul Ha-Yeon Cheong

Department of Chemistry, Oregon State University, USA, United States

A significant number of the most powerful synthetic reactions and materials known today involve compounds that are complex – large in size, complicated in structure, and often exhibiting bewildering flexibility & variability. In many cases, virtually nothing is known or understood about how structure leads to function. Our group's main goal is to expand the reach of theory towards these systems. Together with dozens of research groups around the world, we elucidate mysteries, create predictability, and ultimately bring forth hypotheses that govern complex matter in our effort to augment synthetic organic chemistry efforts by our collaborators. In this seminar, we discuss our latest research into the mechanisms and stereoselectivities of isothiourea Lewis-Base catalyzed reactions, a collaboration with Prof. Andrew Smith group at St. Andrews, UK. We will explore traditional computational as well as new statistical approaches that aid in rationalizing the origins of selectivity and reactivity in these reactions.

Symposium : **ORGN3-1**
Joint Organic Chemistry Symposium: Basic Research Lab
Room 306 (Live Streaming) TUE 15:00
Chair: Jin Kyoon Park (Pusan National University)

Catalytic Enantioselective Cyclopropanation and Tandem Rearrangement

Do Hyun Ryu

Department of Chemistry, Sungkyunkwan University, Korea

The proton-activated chiral oxazaborolidinium ion (COBI) catalyst, which can activate various carbonyl compounds such as aldehydes, ketones, acroleins, and enones through Lewis acid-base interactions and synergistic hydrogen bonds, facilitates asymmetric 1,2- or 1,4-carbonyl additions of nucleophiles. Nucleophilic 1,4-addition of diazo compounds and chemoselective ring-closure afforded an efficient approach to cyclopropanes; and their tandem rearrangements provided four- five and seven-membered cyclic compounds with excellent stereoselectivity. In this talk, our recent studies on COBI-catalyzed enantioselective domino reactions of diazo compounds will be presented. Logical mechanistic explanations of asymmetric COBI catalysis will be also discussed.

Symposium : **ORGN3-2**
Joint Organic Chemistry Symposium: Basic Research Lab
Room 306 (Live Streaming) TUE 15:20
Chair: Jin Kyoon Park (Pusan National University)

Towards New Chemical Space and Tools for Creating Bioactive Molecules

Hyun-Suk Lim[*]**, Kang Ju Lee**

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

After the completion of the human genome project, it is estimated that there are up to 10,000 disease related genes in the human genome. The goal in post-genomic era would be to understand and control the functions of each gene. Therefore, there is an urgent need to develop molecules that can modulate the functions of these disease-related proteins. Such molecules could not only serve as invaluable probes to delineate the protein functions, but also be further developed as therapeutic candidates. However, it is very challenging to deal with overwhelming numbers of target proteins to discover molecules targeting each protein. Furthermore, many proteins (e.g., those that are involved in protein-protein interactions) are not readily targeted by typical small drug-like molecules. Here I will present our chemical approaches to discover such molecules capable of modulating proteins functions, which include the development of new chemical space (suitable for currently undruggable targets), new methods for modulating cellular proteins, and ultra high-throughput screening methods for facilitating rapid identification of protein ligands.

Symposium : **ORGN3-3**

Joint Organic Chemistry Symposium: Basic Research Lab

Room 306 (Live Streaming) TUE 15:40

Chair: Jin Kyoon Park (Pusan National University)

Catalytic reactions for signal amplification in biosensors

Haesik Yang

Department of Chemistry, Pusan National University, Korea

High signal amplification is essential for ultrasensitive detection of biomolecules. In many cases, the signal amplification is based on chemical amplification using the catalytic reactions that are slightly different from the catalytic reactions required in organic synthesis. Catalytic reactions in biosensors should mainly occur in aqueous solutions containing electrolyte and dissolved oxygen. Moreover, the catalytic reactions should not proceed in the absence of catalysts. Therefore, limited catalytic reactions can be used for signal amplification. In this presentation, new catalytic reactions combined with electrochemical detection and redox cycling will be introduced. The developed catalytic reactions are based on a concept that an outer-sphere-reaction-philic species reacts slowly with an inner-sphere-reaction-philic species.

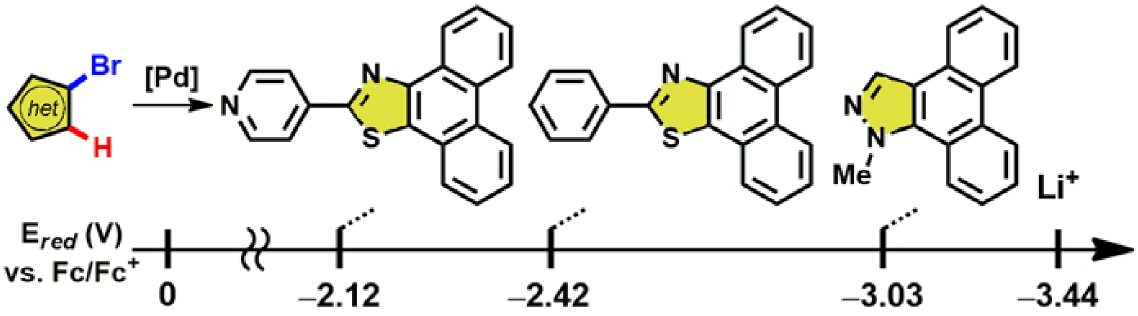
Symposium : **ORGN3-4**
Joint Organic Chemistry Symposium: Basic Research Lab
Room 306 (Live Streaming) TUE 16:00
Chair: Jin Kyoon Park (Pusan National University)

Palladium-Catalyzed C–H Functionalization for the Synthesis of Redox-Active Heteroarenes

Jung Min Joo

Department of Chemistry, Pusan National University, Korea

New methods of synthesizing redox-active heteroarenes by C–H bond functionalization were developed. Pd-catalyzed direct C–H arylation reactions were applied to the annulation of halo- and aryl-heteroarenes with readily available o-bromobiaryls and o-dibromoaryls, respectively. A variety of five-membered heteroarenes, including pyrazole, thiazole, oxazole, thiophene, furan, and pyrrole, rapidly provided the corresponding π-extended structures, which led to the identification of phenanthro-pyrazole and thiazole as new, stable –2 V redox couples. The flexible syntheses and tunability of the redox potentials of these azole-fused phenanthrenes over a wide range is expected to facilitate their application as redox-active organic functional materials.



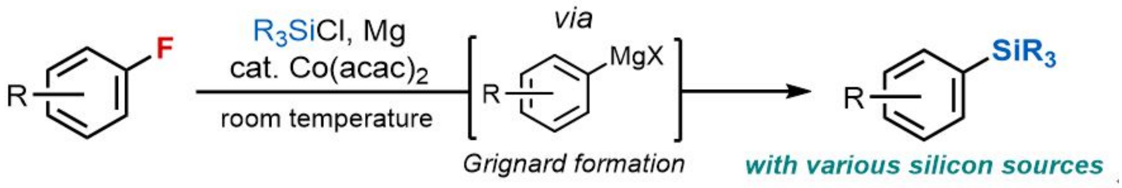
Symposium : **ORGN3-5**
Joint Organic Chemistry Symposium: Basic Research Lab
Room 306 (Live Streaming) TUE 16:20
Chair: Jin Kyoon Park (Pusan National University)

A Simple and Practical Cobalt Catalysis Enabling Grignard Reagent Formation of Aryl Fluorides for Various Organic Transformation

Eunsung Lee

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

Transition metal-catalyzed transformation of C−F bond not only tackles an interesting problem of challenging bond activation, but also offers new synthetic strategies where the relatively inert C–F bond is converted to versatile functional groups. Herein, we report a practical cobalt-catalyzed functionalization of aryl fluorides that uses a cheap electrophilic silicon source with magnesium. This method is compatible with various silicon sources and can be operated under aerobic conditions. Mechanistic studies support in situ formation of a Grignard reagent from the aryl fluoride, which is captured by electrophilic silicon sources. Accordingly, this method not only achieves silylation of aryl fluorides but also allows divergent transformation of aryl fluorides exploiting the common reactivity of the Grignard reagent such as nucleophilic additions or the Kumada coupling.1. (a) Lim, S.; Song, D.; Jeon, S.; Kim, H.; Lee, S.; Cho, H.; Lee, B. C.; Kim, S. E.; Kim, K.; Lee, E. Org. Lett. 2018, 20, 7249. (b) Lim, S.; Cho, H.; Jeong, J.; Jang, M.; Kim, H.; Cho, S. H.; Lee, E. Submitted.



Symposium : **ORGN3-6**
Joint Organic Chemistry Symposium: Basic Research Lab
Room 306 (Live Streaming) TUE 16:40
Chair: Jin Kyoon Park (Pusan National University)

Glycerol Conversion to Value-Added Chemicals

Jung Woon Yang

Department of Energy Science, Sungkyunkwan University, Korea

Glycerol is a triol that can be generated as a by-product during the synthesis of biodiesel from vegetable oils, such as soybean and sunflower oils. Nowadays, there have been made efforts to synthesize renewable materials utilizing biomass derivatives containing overproduced glycerol in industrial research. Glycerol is no longer considered a byproduct of biodiesel production and is recognized as a privileged scaffold due to its potential as a high-value carbon and oxygen source and alternative to our gradually depleting existing natural resources. Therefore, a diverse range of organic transformations are needed for glycerol conversion. Herein, we describe a transition-metal-free chemoselective oxidative dehomologation of 2-*O*-arylmethyl glycerol to give aromatic carboxylic acid and 2-(aryloxy)acetic acid, which represents an unprecedented product pattern, under an oxygen atmosphere.In particular, further transformation of 2-(aryloxy)acetic acid to the unnatural α-amino acid was investigated using potentially infinite natural resources such as sodium and (*S*)-α-amino acids.

Symposium : **MEDI-1**
The Cutting Edge of Medicinal Chemistry
Room 302 (Live Streaming) TUE 13:00
Chair: Chang-Soo Yun (KRICT)

Development of Cenobamate, new hope for treatment-resistant epilepsy

Coomin Chung

Drug Research Center, SK biopharmaceuticals, Korea

Epilepsy is the fourth1) most common neurological disorder characterized by recurrent, unprovoked seizures that have a significant impact on the quality of life (QOL). The goal of treatment is to eliminate seizures with minimal or no adverse events. Antiepileptic drugs (AEDs) are often utilized as the first treatment measure. Despite more than 20 FDA-approved AEDs available for the treatment of epilepsy, recent longitudinal study results showed that newly diagnosed patients with epilepsy still have the same, unchanged outcomes for the past 30 years. Given the relatively static rate of seizure freedom with the current AED armamentarium, an urgent need remains for the development of new compounds to help enable more patients to achieve seizure freedom. Cenobamate is a novel tetrazole alkyl carbamate derivative that has been demonstrated to reduce repetitive neuronal firing by inhibiting voltage-gated sodium currents and as a positive allosteric modulator of the GABAA ion channel. Based on data from pivotal trials that assessed the efficacy and safety in more than 1,900 patients, Cenobamate (XCOPRI®) was approved by the U.S. Food and Drug Administration on November 21, 2019 for treatment of focal onset seizures in adult patients.1)Prevalence : 5~15/1,000

Symposium : **MEDI-2**
The Cutting Edge of Medicinal Chemistry
Room 302 (Live Streaming) TUE 13:40
Chair: Chang-Soo Yun (KRICT)

Small molecules can function like antibodies: Discovery of small molecule TNF-α inhibitors

Kye jung Shin

College of Pharmacy, The Catholic University of Korea, Korea

Cytokines (ILs, TNFα, etc.) and corresponding receptor protein bindings that are part of the stimulatory or inhibitory signaling are critical for cell response and are important therapeutic targets for immunomodulation. Antibody biologics targeting cytokines and their receptors have revolutionized treatment of cytokine-related diseases such as rheumatoid arthritis and Crohn's disease due to their specificity, efficacy, and speed of onset. However, although antibodies have achieved considerable clinical and pharmaceutical success, unmet medical needs are existed in the antibody treatment on the points of cost, non-oral administration, and immunogenicity. To overcome these drawbacks of antibody biologics, many efforts have been carried out to find small molecule drugs that play a same role of antibody.In the last several years, we have focused on finding small molecules that bind directly to TNFα, inhibit the binding of TNFα to its receptors, and modulate its signal transduction pathways in consequence. To date, none of small molecule TNFα inhibitors have made it *in vivo* testing, even though there are some known small molecule scaffolds that have binding affinity to TNFα *in vitro*. In this presentation, we demonstrate that small molecule compounds that bind directly to TNFα could function like TNFα antibodies including *in vitro* and *in vivo* animal experiments.

Symposium : **MEDI-3**
The Cutting Edge of Medicinal Chemistry
Room 302 (Live Streaming) TUE 14:20
Chair: Chang-Soo Yun (KRICT)

Discovery of a First-in-Class RIP1 Kinase Inhibitor GSK2982772

Jaeuk Jeong

Mogam Institute for Biomedical Research, Korea

The recent discovery of the role of RIP1 kinase in TNF-mediated inflammation has led to its emergence as a highly promising target for the treatment of multiple inflammatory diseases. As a part of drug discovery efforts in GSK, a novel benzoxazepinone template from DNA-encoded libraries was identified. This kinase template possessed high RIP1 potency and complete mono-kinase selectivity. Lead optimization focusing on improving lipophilicity, solubility and pharmacokinetic profile, led to identify the highly promising molecules for the clinical studies in psoriasis, rheumatoid arthritis, and ulcerative colitis patients.

Award Lecture in Division : **MAT1-5**
New Horizons in Materials Chemistry
Room 304 (Live Streaming) TUE 11:40
Chair: Hyeon Suk Shin (UNIST)

Perovskite Solar Cell: History, Progress and Perspective

Nam-Gyu Park

Division of Chemical Engineering, Sungkyunkwan University, Korea

Since the seminal report on the 9.7% efficient and 500 h-stable solid-state perovskite solar cell (PSC) in 2012, following two seed reports on perovskite-sensitized liquid junction solar cells in 2009 and 2011, perovskite photovoltaics has been surged swiftly due to high power conversion efficiency (PCE) obtainable via facile fabrication procedure. As a result, a PCE of 25.2% was recorded in 2019. According to Web of Science, number of publications on PSCs increases exponentially since 2012, leading to the accumulated publications of more than 17,500, which indicates that PSC, needless to say, is promising next-generation photovoltaics. High photovoltaic performance was realized by compositional engineering, device architecture and fabrication methodologies for the past 10 years. Toward theoretical efficiency over 30% and commercialization of PSC, further studies on removal of recombination and scalable technologies are required for next 10 years. In this talk, importance of interface engineering is emphasized to reach the theoretical efficiency with voltage over 1.3 V and fill factor over 0.9. Material selection rule and interface engineering methodologies will be introduced. For commercialization, materials may be issued because the current precursor mixture is problematic due to the underlying aging effect. We developed cost-effective materials based on delta FAPbI3 powder for reproducibly high efficiency PSC. Large-area uniform perovskite coating is also important in upscaling PSC. Acetonitrile-based and 2 methoxy ethanol-based coating solutions were developed for large-area perovskite films. In addition, additive engineering and bifacial stamping technique were found to be effective ways for the upscaling PSC. A paradoxical approach is discussed for improving stability of PSCs. PCEs over 23% could be achieved by the interface engineering, the additive engineering and the topographical approach.

Symposium : **MAT1-1**
New Horizons in Materials Chemistry
Room 304 (Live Streaming) TUE 10:20
Chair: Sang Hoon Joo (UNIST)

Crystal engineering of nanocatalysts to achieve both catalyst activity and stability toward water splitting

Kwangyeol Lee

Department of Chemistry, Korea University, Korea

The proton exchange membrane water electrolysis (PEMWE) with advantages of high proton conductivity and low operation temperature has received considerable attention because of its potential as a carbon-zero energy production technology to provide solution to the escalating environmental issues from the usage of fossil fuels. However, the stability issue of catalysts, mostly iridium (Ir) oxide and ruthenium (Ru) oxide based, for the oxygen evolution reaction (OER) in acidic electrolytes remains a formidable roadblock toward a widespread adoption of the PEMWE technology. Through a series of research efforts, we have deciphered that the oxidation state of the metal cations as well as the crystal structure of them are the decisive factors for the catalyst stability, and endeavored to capture the activity and stability of the catalyst simultaneously by engineering these structural features. We found that doping of the catalytic metal oxides by noble metal atoms can establish the desired catalyst stability, while preserving the catalytic activity. In this talk, I will describe our cumulative efforts as a group in the doping of catalytic metal oxides by noble metals for the oxygen evolution reaction. Specifically, I will summarize the most effective strategies as well as method0logy-dependent catalytic performance in order to provide further directions for the field of water splitting with the ultimately goal of spearheading to the future energy landscape with the breakthroughs in PEMWE technology.

Symposium : **MAT1-2**
New Horizons in Materials Chemistry
Room 304 (Live Streaming) TUE 10:40
Chair: Sang Hoon Joo (UNIST)

Novel Plasmonic Nanoarchitectures for Efficient Solar Energy Conversion

Sang Woo Han

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

Solar energy conversion to fuels based on charge carrier generation in semiconductors is a highly evolved scientific and industrial enterprise. Recently, it has been suggested that charge carriers either transferred directly from a photo-excited plasmonic metal nanostructure to an adjacent semiconductor, or induced by the plasmon energy transfer from a plasmonic nanostructure, could boost the efficiency of solar energy conversion processes, leading to a totally new paradigm in harvesting solar energy for practical use. In this context, both the development of a rational strategy that can enable precise control over the topology of heteronanostructures consisting of plasmonic metals and semiconductors and the elucidation of the underpinning mechanism of solar energy conversion processes are highly demanding to fully exploit the plasmonic function of the metal domain in heteronanostructures and thus to devise innovative solar energy conversion platforms. Here recently developed novel synthetic strategies to the realization of plasmonic metal-semiconductor heteronanocrystals with desired configurations and their use in plasmon-enhanced photocatalytic hydrogen evolution are reported. The prepared heteronanocrystals could enable the drastic elevation of solar energy conversion efficiency as well as the elucidation of the underpinning mechanism of the plasmon-enhanced photocatalysis.

Symposium : **MAT1-3**
New Horizons in Materials Chemistry
Room 304 (Live Streaming) TUE 11:00
Chair: Hyeon Suk Shin (UNIST)

Magic Sized Clusters for Nanocrystal Chemistry

Sung Jee Kim

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

Magic sized clusters (MSCs) are thermodynamically stable intermediate nanoclusters often captured during the growth of semiconductor nanoparticles (NPs). MSCs can be isolated as intermediates in quantum dot (QD) synthesis, and they provide pivotal clues in understanding QD growth mechanisms. To investigate the role of MSCs in the nucleation and growth into InP NPs and to find new ways to control the InP NP growth pathways, several heat-up syntheses using the InP 386-MSCs were performed, which resulted in various InP nanostructures including nanorods, pods, hyper-branched NSs and dendrimer-like nanostructures. Highly anisotropic InP structures were obtained without using any structure-directing agents. This demonstrates that sophisticated control over the growth pathways using MSCs offers novel NSs that cannot be attained by conventional synthetic protocols. We also report syntheses for two families of heterogeneous-atom-incorporated InP MSCs that have chlorine or zinc atoms. All the MSCs could be directly synthesized from conventional molecular precursors. Alternatively, each series of MSCs could be prepared by sequential conversions. 386-InP MSCs could be converted to F360-InP:Cl MSCs, then to F399-InP:Cl MSCs. Similarly, F360-InP:Zn MSCs could be converted to F408-InP:Zn MSCs, then to F393-InP:Zn MSCs. As the conversion proceeded, evolution from uni-molecule-like to QD-like characters was observed. Early stage MSCs showed active inter-state conversions in the excited states, which is characteristics of small molecules. Later stage MSCs exhibited narrow photoinduced absorptions at lower-energy region like QDs. The crystal structure also gradually evolved from polytwistane to more zinc-blende.

Symposium : **MAT1-4**
New Horizons in Materials Chemistry
Room 304 (Live Streaming) TUE 11:20
Chair: Hyeon Suk Shin (UNIST)

Multi-Dimensional Liquid Phase TEM for Studying Nanomaterials

Jungwon Park

School of Chemical and Biological Engineering, Seoul National University, Korea

Molecular or atomistic mechanistic understanding of growth and structural changes of materials have not achieved enough at the nanoscale due to a lack of appropriate analytical methods that can obtain in-situ structural information at the nanoscale level. The liquid phase transmission electron microscopy (TEM) offers an opportunity to directly observe chemical reactions that occur in solution. Here we present application of liquid phase TEM to study growth of colloidal nanoparticles. We focus on recent in situ TEM studies of nanoparticle growth which reveal important roles of non-classical crystallization pathways in the entire formation process. Our in-situ observations with liquid phase TEM elucidate different types of non-classical pathway, including two-step nucleation, amorphous-to-crystalline transition, and coalescence of clusters, are involved in different conditions of nanoparticle synthesis. We also present examples of using liquid phase TEM in understanding 3D structures of nanoparticles and phase transformation induced by electrochemical reactions.

Award Lecture in Division : **MAT2-4**
Recent Trends in Photocatalytic Materials
Room 304 (Live Streaming) TUE 14:20
Chair: Tae Woo Kim (KIER)

Molecular designing in carbon-based nanomaterials and their catalytic and optical applications

Sungjin Park

Department of Chemistry, Inha University, Korea

The generation of molecularly dispersed active species on the surface of carbon-based network enables to utilize advantages of molecular catalysts as well as to extremely expose active species without aggregation at the surface. In the first part of this presentation, I will discuss my recent research activities on this concept. Novel hybrids were generated by the reaction of Co-containing organometallic molecules and carbon-based materials. Three dimensional (3D) carbon nitrides (C3N4), which are also referred to as graphitic or polymeric C3N4, have attracted intense research interest because of their visible-light active, fluorescent, biocompatible, and catalytically active properties. In the second part of this presentation, the use of carbon nitride-based materials as photocatalysts and light-emitting materials will be discussed.

Symposium : **MAT2-1**
Recent Trends in Photocatalytic Materials
Room 304 (Live Streaming) TUE 13:00
Chair: Ji-Hyun Jang (UNIST)

Engineering Semiconductor Nanomaterials for Sustainable Photocatalysis

Wonyong Choi

Division of Environmental Science and Engineering, Pohang University of Science and Technology, Korea

The photoinduced electron transfers occurring at the semiconductor surface are the key process of solar photosynthetic and photocatalytic processes. This phenomenon has been extensively investigated for the environmental purification of water and air and the solar energy storage through solar fuel synthesis: the former is photocatalytic and the latter is photosynthetic. Metal oxides semiconductors such as TiO_2, WO_3, and Fe_2O_3 and polymeric carbon nitride ($g\text{-}C_3N_4$) that consist of earth-abundant elements are the most practical base materials for such applications. The semiconductor materials have been employed in the form of nanoparticles for photocatalysis and electrodes for photoelectrochemistry. Although both environmental and energy conversion processes are based on the same photoinduced charge transfer phenomenon, the specific characteristics required for one are very different from the other. While intensive research activities are focused mainly on the development of new photocatalytic materials, the limitations and challenges in photocatalytic research need to be more seriously considered and studied. A variety of approaches have been investigated to modify the base semiconductors and to control the photocatalytic activity and mechanisms using diverse inorganic and organic materials. In this talk, various semiconductor systems with interfacial heterojunctions will be introduced and discussed for photoelectrochemical and photocatalytic/photosynthetic applications. Each research example will be discussed in view of how the modified semiconductor interface affects the photocatalytic activities and mechanisms.

Symposium : **MAT2-2**
Recent Trends in Photocatalytic Materials
Room 304 (Live Streaming) TUE 13:40
Chair: Ji-Hyun Jang (UNIST)

Interface Engineering of Photoelectrodes with Polymeric Materials for Solar-to-Chemical Energy Conversion

Jungki Ryu

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

Electrochemistry can provide an efficient and sustainable route for the production of various chemicals and enable effective use and storage of localized and intermittent renewable energy sources. In principle, various chemicals, such as hydrogen and hydrocarbons, can be produced in an environmentally friendly and carbon-neutral manner using electricity from renewable energy resources or directly using sunlight. However, there remain many challenges that should be addressed for the practical application of solar-to-chemical energy conversion technologies, such as high-cost, low energy efficiency, and poor stability of the conversion systems. In this talk, I will briefly overview recent efforts to address these issues and present our progress over the past few years with a specific focus on interface engineering of photoelectrodes with polymeric materials. In particular, the following topics will be discussed in this talk: (1) immobilization of molecular electrocatalysts on photoelectrodes, (2) modular assembly of various functional components for solar water oxidation, (3) passivation of surface-states and formation of interfacial dipole moments for facile charge separation, and (4) development of superaerophobic surface for efficient removal of gas bubbles using polymeric materials. References)1) D. Jeon et al., ACS Appl. Mater. Interfaces 2017, 9, 40151.2) Y. Choi et al., ACS Nano 2019, 13, 467.3) S. Bae et al., ACS Appl. Mater. Interfaces 2019, 11, 7990.4) S. Bae et al., Adv. Funct. Mater. 2020, 30, 1908492.5) D. Jeon et al., Sci. Adv. 2020, 6, eaaz3944.

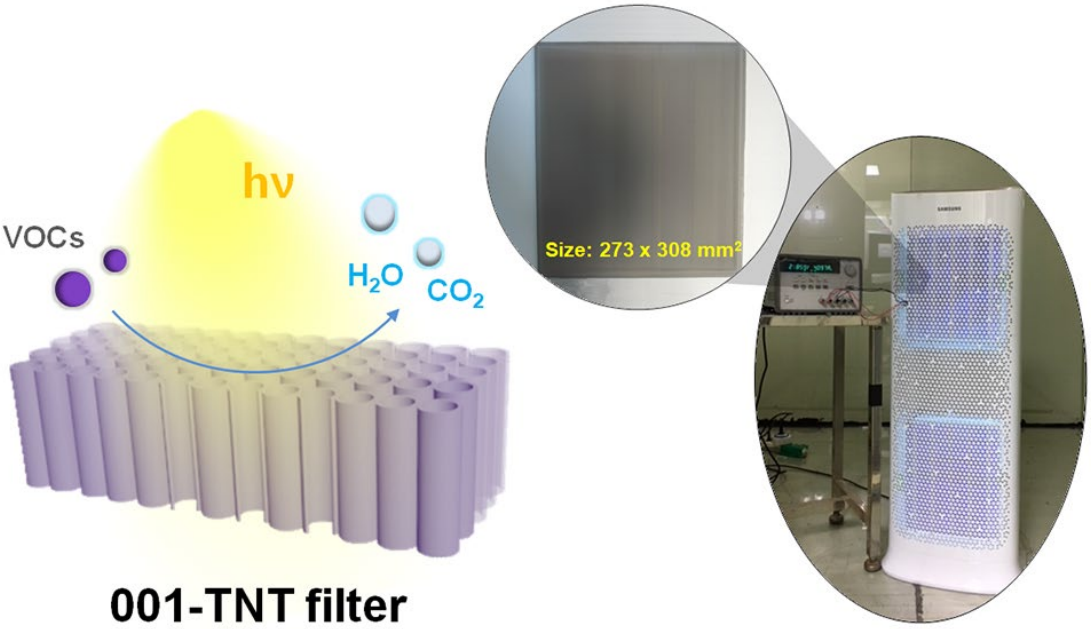
Symposium : **MAT2-3**
Recent Trends in Photocatalytic Materials
Room 304 (Live Streaming) TUE 14:00
Chair: Tae Woo Kim (KIER)

Status and Challenges in Photocatalytic Air Purification: From Material Development to Air Cleaner Application

Seunghyun Weon

School of Health and Environmental Science, Korea University, Korea

The leading technology for removing indoor air pollutants is the adsorption using filtration media such as activated carbon. However, it is doubtful whether the adsorption technology is efficient since removal efficiency of adsorbents is remarkably reduced on humid condition. In addition, adsorbed air pollutants can be re-emitted from the media to ambient air. Photocatalytic air purification technology is a promising method for removing indoor volatile organic compounds (VOCs) because it can degrade VOCs completely to harmless CO2 and H2O under ambient conditions. In this talk, the principles of photocatalytic air purification, various physicochemical modifications of photocatalysts (Nanotubes structures, metal loading, surface fluorination, and exposed facets), and success case of photocatalytic air cleaner will be introduced.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VOCs
H_2O
CO_2
001-TNT filter
Size: 273 x 308 mm²

Symposium : **MAT3-1**
Recent Trend in Next-Generation Optoelectronics
Room 304 (Live Streaming) TUE 15:00
Chair: Hyosung Choi (Hanyang University)

Strategic Approaches for Efficient Doping of Conjugated Polymers: Catalytic Cascade Doping and Hybrid Doping Porcesses

Jong Hyun Kim

Department of Molecular Science and Technology, Ajou University, Korea

In this talk, general background of molecular doping is introduced and a newly developed efficient molecular doping approaches for preparing highly conductive conjugated polymer films will be presented.

Symposium : **MAT3-2**
Recent Trend in Next-Generation Optoelectronics
Room 304 (Live Streaming) TUE 15:20
Chair: Hyosung Choi (Hanyang University)

Ligand engineered bandgap stability in mixed-halide perovskite nanocrystals light-emitting diodes

Bo Ram Lee

Department of Physics, Pukyong National University, Korea

Lead halide perovskites are promising semiconductors for light-emitting applications, owing to their bright, bandgap tuneable and high colour purity luminescence. Close to unity photoluminescence quantum yields have been achieved for perovskite nanocrystals across a broad range of emission colours, and light emitting diodes with external quantum efficiencies exceeding 20%, which approach commercial OLEDs, have been demonstrated in both the Infrared and green emission channels. However, due to the formation of lower bandgap iodide-rich domains in mixed-halide perovskites, achieving colour-stable and efficient red electroluminescence at the desired wavelength is yet to be realised. Here, we report mixed-halide perovskite nanocrystals passivated with multidentate ligands that suppress halide segregation, under electroluminescent operation. We demonstrate colour-stable red emission centred at 620 nm, with electroluminescence external quantum efficiencies of 20.3% in light emitting diodes. We use Density Functional Theory to model the nature of binding between the ligands and the nanocrystal surface, which we find suppresses iodine Frenkel defect formation, and infer inhibits halide-segregation. Our work exemplifies how the functionality of metal halide perovskites is extremely sensitive to the nature of the (nano)crystalline surface and presents a route for controlling surface defect formation and migration. This is critical for achieving band gap stability for light emission and will also have a far-reaching impact for other optoelectronic applications, such as photovoltaics, where bandgap stability is required.

Symposium : **MAT3-3**
Recent Trend in Next-Generation Optoelectronics
Room 304 (Live Streaming) TUE 15:40
Chair: Hyosung Choi (Hanyang University)

CNT-incorporated Nickel Oxide hybrid charge collectors for Planar Perovskite Solar Cells

Dong-Won Kang

Energy Systems Engineering, Chung-Ang University, Korea

In this study, we employed simple solution processes to prepare a hybrid material consisting of carbon nanotubes embedded in NiOx. The addition of carbon nanotubes improved the conductivity of the metal oxide but did not significantly affect its advantageous optical and morphological characteristics. Applying the hybrid material as a hole transport layer in inverted planar perovskite solar cells (PSCs) enhanced the average power conversion efficiency (PCE) from 14.3% to 15.6%, with the best performing cell exhibiting a PCE of 16.2%. We believe that our study makes a significant contribution in this field because this unprecedented method for improving the properties of NiOx hole transport layers and device performance could be expanded to enhance the conductivity of other oxide materials for inverted planar PSCs.

Symposium : **MAT3-4**
Recent Trend in Next-Generation Optoelectronics
Room 304 (Live Streaming) TUE 16:00
Chair: Jong Hyun Kim (Ajou University)

Internal Quantum Efficiency of Solar Cells with Organic and Quantum Dot Absorbers through Optical Simulation

Hyeok Kim

University of Seoul, Korea

The internal quantum efficiency (IQE) of a solar cell is the ratio of the number of charge carriers extracted from the cell to the number of photons absorbed in the active layer of the solar cell. The IQE value of a solar cell can provide us useful information about electrical properties of the solar cell because IQE measurements normalize the current generation efficiency by photon generation efficiency and separates the electrical properties from optical properties of the solar cells. In a solar cell the magnitude of the IQE is inversely proportional to the probability of charge carrier recombination in the cell. The wavelength dependent IQE spectra of a solar cell can also provide information about exciton harvesting efficiency of the cell and spatial dependence of charge recombination [1]. Presence of many other interesting effects such as multiple exciton generation, singlet exciton fission, and bias-dependent photoconductivity within a solar cell can also be detected by measuring IQEs greater than 100% [2-3]. Despite its usefulness as a characterization tool, IQE is rarely reported due to the unavailability of its estimation method. For the accurate estimation of IQE value of a solar cell, we need to utilize the absorption spectra of active layer of the cell. The active layer exists within the cell so it is not possible to record the absorption spectra of the active layer of the solar cell directly [4]. When IQE is reported, absorption is frequently not measured in actual devices; this can lead to errors since reflective electrodes induce strong interference effects that substantially affect absorption. When absorption is measured in actual devices, parasitic absorptions are almost never taken into account. Therefore, here, we have utilized optical simulation as a tool to estimate the absorption spectra of the active layer of different solar cells (organic and quantum dot) more precisely. To describe the optical properties of different layers of those solar cells we have incorporated frequency dependent refractive index (n) and extinction coefficient (k) values of those layers in the software interface. Afterwards, we have used the estimated absorption spectra of active layers of different solar cells and experimentally measured external quantum efficiency (EQE) of those cells to estimate their IQE spectra.

We believe that this straightforward method of measuring IQE will help the community to understand the underlying mechanism behind high performance solar cells.References 1.G. F. Burkhard, E. T. Hoke, M. D. McGehee, Nano Lett. 9, 4037 (2009). 2.R. D. Schaller, V. I. Klimov, Phys. Rev. Lett. 92, 186601 (2004).3.A. J. Nozik, Physica E. 14, 115 (2002).4.M. Law et al., Nano Letters. 8(11), 3904 (2008).

Symposium : **MAT3-5**
Recent Trend in Next-Generation Optoelectronics
Room 304 (Live Streaming) TUE 16:20
Chair: Jong Hyun Kim (Ajou University)

Development of conjugated cathode buffer layer materials for photodiode applications.

In Hwan Jung

Department of Applied Chemistry, Kookmin University, Korea

The p-n junction photodiodes have widely utilized in solar cells and image sensors, and the high-efficiency photodiodes are achieved by the suppression of leakage current and charge recombination and the improvement of photo-induced charge collection. In this study, the conjugated polyelectrolytes and high dipole small molecules were designed and synthesized to improve the photo-induced current density and reduce the dark current density in the devices as a cathode buffer layer. The synthesized cathode buffer layer materials was coated on the electron transporting layer (ETL), which dramatically enhanced the photodiode properties via modifying the work function of the ETL and improving the surface contact properties between ETL and active layer. The detailed discussion will be given in the presentation.

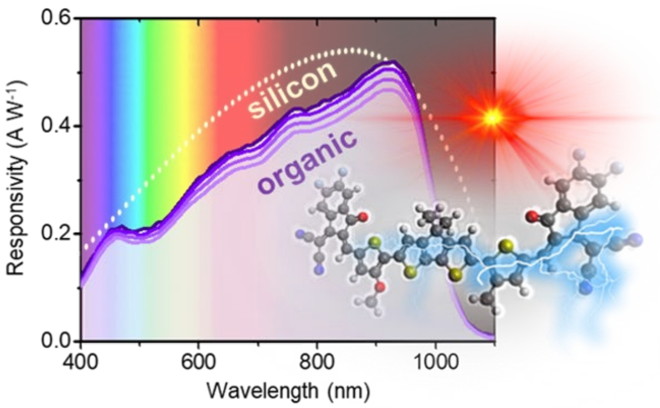
Symposium : **MAT3-6**
Recent Trend in Next-Generation Optoelectronics
Room 304 (Live Streaming) TUE 16:40
Chair: Jong Hyun Kim (Ajou University)

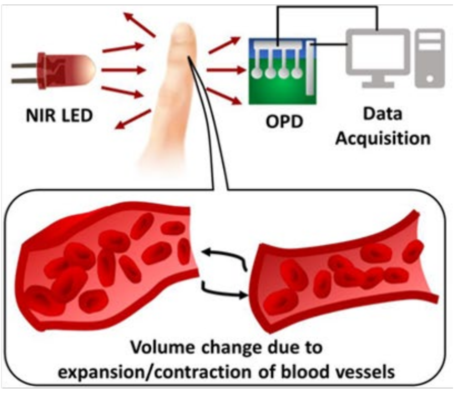
Near Infrared Responsive Fullerene-Free Organic Solar Cells and Photodetectors Based on Narrow Bandgap Bulk Heterojunction Blends

Jaewon Lee

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Korea

Narrow bandgap organic semiconductors are relevant as key materials components for the fabrication of near-infrared (NIR) organic solar cells (OSCs) and organic photodetectors (OPDs). Much of the interest arises due to the tunability of their energy levels and absorption properties through designing the molecular architecture. However, the benefits of NIR organic semiconductors remain comparatively unexplored in the context of OSCs and OPDs. A critical challenge arises as one decreases optical bandgaps (Egopt) with respect to the counterbalance between the driving force for charge separation and voltage loss in the solar cell devices. We thus designed and synthesized narrow bandgap nonfullerene acceptors (NFAs), which exhibit thin film absorbances that span from 600 nm to 1100 nm. As a preliminary assessment of NIR light sensing as a practical application, we carried out a simple photoplethysmography (PPG) test using our OPDs. The present OPDs could achieve a high maximum responsivity over 0.5 A W-1 in the NIR region beyond 900 nm, marking one of the highest responsivity achieved by organic photodiodes in the NIR spectrum.





Award Lecture in Division : **ELEC1-1**

Computationl Electrochemistry

Room 408 (Live Streaming) TUE 11:00

Chair: Byung-Kwon Kim (Sookmyung Women's University)

Controls the electrolyte-water interaction for LiCoO2 to improve the performance of aqueous lithium-ion batteries and oxygen evolution catalysts

Hye Ryung Byon

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

Layered lithium cobalt oxide (LiCoO2) was developed by Professor John Goodenough in 1980 and was commercialized as the first lithium-ion batteries (LIBs) in 1981. LiCoO2, which has been studied for a long time, is a very familiar material. There is nothing more to study, but little is understood for interfacial electrochemical reaction with water. Here I first discuss the anion-water interaction on the LiCoO2 electrode in aqueous LIB and its effect on the inhibition of water poisoning of LiCoO2, which is a major cause of poor cyclability. Next, I talk about the cation-water interaction when LiCoO2 acts as a catalyst for the oxygen evolution reaction. These two chapters highlight the importance of understanding interfacial reactions and show that controlling electrolyte-solvent interactions can significantly improve cell and catalyst performances.

Symposium : **ELEC1-2**
Computationl Electrochemistry
Room 408 (Live Streaming) TUE 13:00
Chair: Hyungjun Kim (KAIST)

Engineering of cation stability for highly stable and active perovskite-based SOFC electrode materials

Jeong Woo Han

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

Perovskite-based oxides have been widely used to electrode materials in solid oxide fuel cells (SOFCs). However, rearrangement of cations (e.g., segregation and ex-solution) affects the activity and stability of SOFC under operating conditions. Under cathodic (oxidizing) environments, the A-site cation segregation significantly degrades perovskite-based cathode materials in SOFC because segregated Sr atoms form insulating SrOx phases. On the other hand, B-site cation segregation (ex-solution) under anodic (reducing) environments increases the catalytic activity and stability of perovskite-based anode materials in SOFC because the segregated B-site cations act as catalytic sites. Interestingly, both phenomena are commonly related to the breaking of cation-oxygen bonds in oxide materials for the cation's segregation toward the surface. Therefore, controlling of cation-oxygen bond strength is an effective way to engineer cation segregation for designing the highly stable and active electrode materials in SOFC. In this presentation, we first introduce how to understand A-site and B-site cation stability in perovskite materials at the atomic scale using density functional theory (DFT) calculations with the experimental validations. Then, we demonstrate the application of cation stability, such as iso-valent doping, to practically control cation stability in perovskite materials to improve the activity and stability of SOFC electrode materials.

Symposium : **ELEC1-3**
Computationl Electrochemistry
Room 408 (Live Streaming) TUE 13:25
Chair: Hyungjun Kim (KAIST)

An in-depth understanding of electrochemical interfaces through multiscale modeling approach.

Hyung-Kyu Lim*, **Hyungjun Kim**[1,*]

Division of Chemical Engineering and Bioengineering, Kangwon National University, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

The electrified solid-liquid interface system is a core physicochemical component that existed in many types of electrochemical heterogeneous catalyst systems related to various energy and environmental applications, such as fuel-cell, lithium-ion battery, etc. Despite its widespread use in a variety of commercial applications, the detailed physicochemical understanding is still at an early stage due to the difficulty of analysis. From the recent rapid advances in computational hardware and software, the multi-scale simulation framework which utilizes both quantum and molecular mechanics modeling methods is a useful tool to analyze the complex electrified solid-liquid interface system in atomic/molecular-scales. In this presentation, I would present recent research results about understanding the electrified solid-liquid interface systems using own-developed multi-scale simulation frameworks, DFT-CES, such as electrochemical CO_2 conversion, fuel-cell catalyst, and electrical double layer phenomena, etc.

Symposium : **ELEC1-4**
Computationl Electrochemistry
Room 408 (Live Streaming) TUE 13:50
Chair: Hyungjun Kim (KAIST)

Computational study on the materials for rechargeable batteries using first-principles calculation

Dong-Hwa Seo

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

Electrochemical energy storage devices are attracting tremendous interest due to the recent growing importance of sustainability and environmental concerns. The lithium rechargeable batteries are one of the most advanced energy storage systems and serve as a major power source for various small electronic devices. With the growing interest in power sources for large applications such as the HEV (hybrid electric vehicle) or PHEV (plug-in hybrid electric vehicle), lithium rechargeable batteries are finding new opportunities in this emerging area. Intensive research efforts are focused on developing suitable electrode material, the key component of lithium rechargeable battery, for these applications. The new electrode materials for lithium rechargeable battery for use in HEVs and PHEVs requires high stability, high power, high energy and low cost. In this talk, I will present the first-principles results on the oxygen redox activity in Li-excess cathode materials [1] and the reaction mechanism of Li4+xTi5O12 anode materials [2]. Fundamental understanding on the electrode's properties based on first principles can accelerate to develop new electrode materials. References[1] D.-H. Seo et al., "The structural and chemical origin of the oxygen redox activity in layered and cation-disordered Li-excess cathode materials", Nature Chem., 8 692 (2016) [2] D.-H. Seo et al., "Kinetic Pathways of Ionic Transport in Fast Charging Lithium Titanate", Science, 367 (6481) 1030 (2020)

Symposium : **ELEC1-5**
Computationl Electrochemistry
Room 408 (Live Streaming) TUE 14:15
Chair: Hyungjun Kim (KAIST)

First-Principles Catalyst Design at Electrified Solid-Liquid Interfaces

Stefan Ringe

Energy Science & Engineering, DGIST, Korea

Electrocatalysis at electrified solid-liquid interfaces is the key to sustainable storage and conversion of energy. In the search for more active electrocatalysts, first-principles calculations based on Density Functional Theory have become state-of-the-art means, which, however generally, ignore the presence of the interface. In this talk, we revisit the implications of this approximation at the example of electrocatalytic CO_2 reduction. In contrast to previous believes, we find the interfacial electric field to be significant and even determine the product selectivity and conversion rate on Gold and Copper catalysts. From experimental and theoretical studies, we then derive novel interface-aware design principles and apply them for material and electrical engineering towards highly optimized energy conversion systems. We also use the concepts to initiate a descriptor-based screening of catalyst materials for CO_2 reduction and highlight critical differences to previous studies. Finally, we extend the approach by including also mass transport effects which enables the design of electrode materials on all relevant time and size scales.

Symposium : **ELEC2-1**
Electrocatalysis for energy conversions
Room 408 (Live Streaming) TUE 15:00
Chair: Chang Hyuck Choi (GIST)

Designing Atomically Dispersed Electrocatalysts for Controlling Catalytic Selectivity

Sang Hoon Joo

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

The control of catalytic selectivity plays a pivotal role in electrocatalytic reactions to produce desired products. In this presentation, we present the design of electrocatalysts comprising atomically dispersed active sites, which enable selective oxygen reduction reaction (ORR) and chlorine evolution reaction (CER). We developed a general synthetic strategy that can produce atomically dispersed precious metal catalysts (Os, Ru, Rh, Ir, and Pt), which served as model catalysts for unraveling catalytic trends for the ORR. The atomically dispersed precious metal catalysts showed higher selectivity for H_2O_2 production than their NP counterparts for the ORR owing to their isolated geometry. Among the atomically dispersed catalysts, the H_2O_2 selectivity was changed by the types of metals, with atomically dispersed Pt catalyst showing the highest selectivity. The selectivity trend of atomically dispersed catalysts could be correlated to the binding energy difference between *OOH and *O species. For the selective CER, we found that atomically dispersed $Pt-N_4$ sites doped on a carbon nanotube (Pt_1/CNT) can catalyze the CER with excellent activity and selectivity. The Pt_1/CNT catalyst showed superior CER activity to a Pt nanoparticle-based catalyst and a commercial Ru/Ir-based metal oxide catalyst. Notably, Pt_1/CNT exhibited near 100% CER selectivity in acidic media with low Cl^- concentrations (0.1 M) as well as in neutral media, whereas the MMO catalyst showed substantially lower CER selectivity.

Symposium : **ELEC2-2**
Electrocatalysis for energy conversions
Room 408 (Live Streaming) TUE 15:25
Chair: Chang Hyuck Choi (GIST)

I. Bio-inspired Molecular Electrocatalysts and II. Hetero-Metal Oxides Electrocatalysts

Junhyeok Seo

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

Hydrogenases are metalloenzymes that involve in energy metabolisms of microorganisms as promoting the reversible H_2 generation/oxidation reactions. As an effort to develop energy conversion electrocatalyst, hydrogenases-inspired molecular complexes have been synthesized. For example, [FeFe]-hydrogenase promotes electrocatalytic hydrogen reaction, and the active site is known to have a diiron catalytic center assisted by two functional sites for electron-transfer and proton-relay in the secondary coordination sphere. Recently, we synthesized molecular complexes mimicking the enzyme active site by installing a proton-relay functional group in electrocatalytic complexes. In this talk, our current synthetic strategies for bio-inspired molecular electrocatalysts will be discussed.Also, we are interested in nanomaterials surfaces, reactive for (photo)electrochemical reactions. As a research approach, we focus on Group X hetero-metal oxides and investigated their (photo)electrochemical reactivities for the oxygen evolution reaction. In recent studies, we have found that co-fabricated hetero-metal oxides systematically increase oxygen evolution performances as follows: $NiO \rightarrow PdO+NiO \rightarrow PtO_x+NiO$, and their depositions on nanostructured TiO_2 photoanode enhance photoelectrochemical oxygen evolution activities. Moreover, upon combination with perovskite $GdFeO_3$, the PtO_x+NiO nanoparticles exhibited bifunctional electrocatalytic activities for the oxygen evolution and oxygen reduction reactions. In the second part, the various reactivities of Group X hetero-metal oxides will be discussed.

Symposium : **ELEC2-3**
Electrocatalysis for energy conversions
Room 408 (Live Streaming) TUE 15:50
Chair: Chang Hyuck Choi (GIST)

Surface Engineering to Improve Electrocatalytic Performances of Nanocatalysts

Sang-Il Choi

Department of Chemistry, Kyungpook National University, Korea

The catalyst surface has been designed to accelerate or inhibit the rate of oxidation/reduction of chemicals to obtain the desired products. Recently, various nanoscale catalysts have been developed, and studies on chemical reactions on their surfaces have been extensively conducted. In this presentation, the modification of nanosurface to accelerate the rate of core reactions for renewable energy systems will be discussed. In particular, highly improved ammonia oxidation and oxygern evolution reaction activities will be introduced when using nanocatalysts with surface dopants.

Symposium : **ELEC2-4**

Electrocatalysis for energy conversions

Room 408 (Live Streaming) TUE 16:15

Chair: Chang Hyuck Choi (GIST)

Electrocatalytic CO_2 Reduction for Value-added Chemical Production

Dae-Hyun Nam

Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea

Electricity-powered CO_2 conversion to renewable fuels and chemical feedstocks offers a pathway to solve fossil fuel-derived energy and environmental issues. At the heart of this reaction is heterogeneous electrocatalysts; a material which can activate the substrate species, induce proton/electron transfer, control the binding of reaction intermediates, and promote the CO_2 conversion toward target products. Electrocatalytic performance can be affected by the bindings between the reaction intermediates and the surface of electrocatalysts.In this talk, I will present recent progress and research trend for electrochemical CO_2 reduction reaction (CO_2RR). The contents of the presentation will cover from catalyst design to electrolyzer; heterogeneous electrocatalysts to steer the CO_2RR pathway, electrochemical reactors for CO_2RR such as flow cell and membrane-electrode-assembly (MEA) cell, and in-situ spectroscopy to track the behavior of active materials and intermediate binding in real time. As a concluding remark, the future perspective of the electrochemical CO_2RR will be discussed.

Symposium : **ENVR-1**
Electrode and Energy Storage Technology
Room 302 (Live Streaming) TUE 10:20
Chair: Wooyul Kim (Sookmyung Women's University)

Electrocatalytic Hydrogen Cycle for Energy and Environment

Youngkook Kwon

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

The electrocatalytic hydrogen cycle with carbon and nitrogen resources is of emerging interest for renewable energy and environment. Currently, my research focuses on developing efficient and high-performing electrocatalysis system for carbon and nitrogen mediated hydrogen cycle via 1) designing reactive and selective electrocatalysts and electrolytes, 2) fabricating atomic- to large-scale electrode and system, and 3) developing on-line analytical techniques to identify reaction intermediates and products.In this talk, I'll introduce recent works of electrocatalytic conversion of CO2 and NO and future research direction.

Symposium : **ENVR-2**

Electrode and Energy Storage Technology

Room 302 (Live Streaming) TUE 10:50

Chair: Wooyul Kim (Sookmyung Women's University)

Advanced green ammonia synthesis for renewable hydrogen energy storage and carrier by ambient electrochemical route

HyungKuk Ju

Energy, CSIRO, Australia

Hydrogen is considered as a next generation source of energy which has potential to replace fossil fuels and ammonia is considered as the best carrier of hydrogen for energy storage and transport. Recently, the low temperature, ambient pressure, and electrochemical synthesis of ammonia has attracted significant attention as a low energy and renewable alternative to synthesize ammonia compared to energy intensive high-temperature/-pressure conventional process of producing ammonia by the "Haber Bosch" process. Electrochemical synthesis at low temperature and ambient pressure (< 100'C and < 1 bar) offers significant advantages over Haber-Bosch process which involve high temperatures of ~500'C and ~200 bars pressure. However, electrochemical synthesis route's wide adoption has hindered due to the poor yield arising from the ineffective catalysts and their long-term stability. If successfully developed, this green ammonia production process can be the Holy Grail technology for decentralized production of ammonia with green electricity from renewable energy sources to substantially reduce the carbon footprint. Therefore, there is strong need to discover new catalysts and new material which can offer stable and high yield of ammonia production.

Symposium : **ENVR-3**
Electrode and Energy Storage Technology
Room 302 (Live Streaming) TUE 11:10
Chair: Wooyul Kim (Sookmyung Women's University)

Recycling spent lithium ion batteries and their impurity effects

Sungyool Bong

School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Korea

As lithium-ion batteries continuously increase the energy market portion, recycling of Li-ion batteries (LIBs) will ask for regulations due to limited resources. With the demand increment of battery recycling, understanding of impurity is always a concern for LIB recycling since it could work in different forms corresponding to different recycling processes. In addition, as identification and development of lithium-ion battery recycling technologies can be required, understanding the role of impurities is a critical issue, which might be impacted on battery performance, material stabilization, or lifetime for recovered active materials. Herein, we confirmed that copper impurity in different forms could be applied for very different roles on the recovered NCM622. Copper metal impurity can be easily short the cell. In contrast, Copper ion impurity could act as a positive factor since this copper ion partially substituted into the Ni^{2+}sites for lower the cation mixing degree. These positive results clearly explain that copper impurity might be avoided and it should be controlled with optimal concentration during the recycling process for spent LIBs corresponding to the amount of its impurity.

Symposium : **ENVR-4**

Electrode and Energy Storage Technology

Room 302 (Live Streaming) TUE 11:30

Chair: Wooyul Kim (Sookmyung Women's University)

Inactivation induced degradation of a Li-metal electrode for next generation batteries

Jung-Je Woo

Gwangju Bio/Energy R&D Center, Korea Institute of Energy Research, Korea

The high theoretical capacity (3862 mAh/g) and low electrochemical potential of the Li electrode makes it an ideal anode for high energy density of batteries. In the case of novel battery types, such as Li-air and Li-sulfur cells employing a Li-free cathode, Li-metal is in fact considered to be the most promising anode material. However, despite its desirable properties, the Li electrode is rarely used in practical rechargeable batteries due to its poor cycle life and safety issues. In this study, the degradation of the lithium (Li) electrode was investigated based on its structural transformation. Depletion of active Li turned out to be the major reason for the failure of the Li electrode under our experimental conditions. The voltage profile and EIS of the symmetric cell could be correlated with the degradation behavior exhibited by the Li electrode.

Symposium : **ENVR-5**
Electrode and Energy Storage Technology
Room 302 (Live Streaming) TUE 11:50
Chair: Wooyul Kim (Sookmyung Women's University)

Exploring selective, efficient 2 e- electrochemical oxygen reduction at reduced graphene oxide electrocatalysts

Hyo Won Kim

Department of Advanced Materials Engineering, Kangwon National University, Korea

Generally the electroreduction of oxygen can proceed through one of two overall reactions: a 4e- process to convert from O2 to H2O, and a 2e- process to form H2O2. There is general agreement that certain carbon defects selectively catalyze the more thermodynamically favored 4e- mechanism over the 2e- process. However, there is still no consensus regarding the role of each site on the ORR mechanism. In this study, we use a straightforward, low temperature and pressure procedure to synthesize reduced graphene oxide (rGO) and compare the resultant materials' electrocatalytic behavior with rGO and nitrogen doped rGO (N-rGO). To study ORR chemistry, we have characterized electrocatalytic selectivity by monitoring O2 pressure decay in well-stirred, modified electrochemical H-cells with a calibrated, known headspace volume. We also quantify H2O2 formation using a standard iodometric titration on the electrolyte. These techniques provide direct measurements of O2 consumption and H2O2 formation during ORR and are therefore more accurate than traditional rotating ring disk electrode measurements. We have found that certain variants of N-rGO and rGO display exceptionally selective (~100%) and efficient (nearly no onset overpotential) formation of H2O2 in basic conditions. Detailed results will be discussed linking the selectivity and efficiency of the oxygen reduction reaction to the role of distribution of carbon defects in N-rGO and rGO.

Symposium : **EDU-1**
Current Issues and Research in Chemistry Education
Room 302 (Live Streaming) TUE 15:00
Chair: Seounghey Paik (Korea National University of Education)

Development of Computer-Based Evaluation System(KICE-eAssessment) for Core Competency Evaluation

Insuk Kim[*], **Hyun Jung Kim**[1], **Sungki Kim**[*]

Korea Institute for Curriculum and Evaluation, Korea
[1]*Chemistry Education, Kongju National University, Korea*

Recently, as interest in core competencies has increased, evaluation of these is also emerging as important. Paper-based evaluation has limitations in evaluating competencies, and computer-based evaluation has been introduced domestically and internationally to overcome these limitations. Accordingly, KICE has been conducting research on computer-based evaluation system for competency from 2019. And it developed computer-based evaluation system for scientific problem solving ability in 2019. This year, the evaluation system for scientific inquiry ability was developed. The evaluation unit is the characteristics of the material in the second grade of middle school. In addition, an integrated evaluation system has also been developed. Meanwhile, the perception of current chemistry teachers' competency evaluation was examined. The evaluation system developed by KICE is expected to provide practical help for science teachers to evaluate students' competencies.

Symposium : **EDU-2**
Current Issues and Research in Chemistry Education
Room 302 (Live Streaming) TUE 15:20
Chair: Seounghey Paik (Korea National University of Education)

Implementation of Process-Fortified Assessment in Chemistry Classes

Hyun jung Kim

Chemistry Education, Kongju National University, Korea

In the 2015 revised curriculum, in order to cultivate creative·convergence-type people, we emphasized process-fortified assessment evaluation and emphasized the improvement of classes that can foster competencies in the future society. The process-fortified assessment is to elicit positive changes in education through changes in evaluations made in the school field. Based on the achievement standards of the curriculum, the learning is evaluated by maintaining consistency in teaching and evaluation, and it is to evaluate the learning process as well as the outcome of learning. In this study, I would like to discuss the implementation of process-fortified assessment in the field. To this end, the school evaluation plan and inquiry report of 185 chemistry teachers who participated in the training of chemistry teachers at two institutions in August 2020 were analyzed. Among the total evaluations, the percentage of performance evaluation, the number of performance evaluations in the first semester, and the number of experiments were analyzed.To analyze the competencies mainly measured in performance evaluation conducted by schools, evaluation elements were classified using the national academic achievement evaluation framework. As a result of the analysis, among the various sub-elements of science subject competency, a few elements were mainly used for evaluation, and several evaluation elements were not used for evaluation.

Symposium : **EDU-3**
Current Issues and Research in Chemistry Education
Room 302 (Live Streaming) TUE 15:40
Chair: Seounghey Paik (Korea National University of Education)

Argument-based Inquiry in Chemistry Education

Jeonghee Nam

Department of Chemical Education, Pusan National University, Korea

The role of argumentation in science education cannot be overemphasized. This has the same meaning in chemistry education. In chemistry education, various approaches have been used to encourage student argumentation. I will introduce three different approaches based on Argument based Inquiry (ABI), such as Assessment-based ABI that emphasized assessment as a way to activate it, Modeling-based ABI, and Character competence-based ABI. Also I will examine the effects of implementing ABI at the elementary, secondary, and college level.

Symposium : **EDU-4**
Current Issues and Research in Chemistry Education
Room 302 (Live Streaming) TUE 16:10
Chair: Seounghey Paik (Korea National University of Education)

Hybrid models of learning and Teaching

HyunJu Park

Faculty of Science Education, Chosun University, Korea

The purpose of this study was to investigate hybrid learning and teaching model that utilizes technology when direct class is difficult, such as in a COVID-19 situation. The case studies of online classes in Korea and other countries were analyzed, and the actual conditions of online classes used in Korean schools were investigated. Hybrid learning/teaching is an educational model where some students attend class in-person, while others join the class virtually from home. Teachers teach remote and in-person students at the same time using various digita ICT tools like internet or video conferencing hardware and software. Flipped learning with app, active leaning with smart board, collaborative learning by online coachig were proposed.

Symposium : **EDU-5**
Current Issues and Research in Chemistry Education
Room 302 (Live Streaming) TUE 16:30
Chair: Seounghey Paik (Korea National University of Education)

Search for new strategies to strengthen the ability of pre-service chemistry teachers to conduct practical experiment

Jaehyeok Lee, Seounghey Paik[1,*]

Chemistry Education, Korea National University of Education, Korea
[1]Department of Chemical Education, Korea National University of Education, Korea

In order to cultivate the ability of pre-service teachers to teach the experiment, the practical education system of the teacher training college is very poor. Therefore, there is a need for a plan to improve pre-service teacher education, and to establish a support system to actively respond to educational changes in the field. As an example of the plan, it is proposed to operate a science laboratory center in each teacher training college. As in the operation of the gifted education center, a certain amount of subsidies are given to the teachers' colleges and the dispatched teachers are officially provided to develop and operate an experimental education program with professors and pre-service teachers. In the form of a experiment support group at Korea National University of Education, a graduate student and pre-service teachers developed experimental programs for one semester and supported educational services in the Seo-Jeon High School students. Through the operation of this experiment support group, in-depth inquiry that students want to explore was possible, and the actualization of the experimental class became possible. In addition, it was confirmed that the evaluation of the students' inquiry experiment abilities were faithfully carried out. The ability of pre-service teachers to teach the experiment instruction was improved. It is urgent to establish a system for supporting these new types of experimental classes for students and pre-service teachers.

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

Oral Presentation for Young Polymer Scientists

Room 402 (Live Streaming) TUE 09:00

Chair: Seung Goo Lee (University of Ulsan)

Incorporating smart manufacturing in polymer extrusion process

Sunyong Kwon*, Jungup Park, Tae-Jin An, SungHwan Cho*

Chemicals R&D Center, Samyang Corporation, Korea

The manufacturing of engineering plastic involves polymer processing such as extrusion and injection molding. Depending on the different processing conditions (feed rate, temperature, torque, shear stress etc.) and the materials (polymer resin, additives, filler etc.) used in the process, we can produce end products with various shapes and characteristics. In order to keep track of various operating conditions, manufacturing plants have implemented data storage system such as manufacturing execution systems (MES) and real-time database (RTDB). In order to acquire information from these datasets, numerical analysis and machine learning method are applied in this study. We correlated two separate datasets together; operating conditions of the plant from RTDB and final product properties from MES. After merging these two datasets, we applied machine learning techniques to predict the properties of plastic compound and detect defective products.

Oral Presentation : **POLY.O-2**
Oral Presentation for Young Polymer Scientists
Room 402 (Live Streaming) TUE 09:20
Chair: Seung Goo Lee (University of Ulsan)

Ionic conductors using chemically linked ionic side chains and applications to thermally stable actuators and sensors

Junwoo Lee, Taehyun Kim, Dasol Chung[1], Dohyun Kim[2], Taiho Park[*]

Department of Chemical Engineering, Pohang University of Science and Technology, Korea
[1]*Pohang University of Science and Technology, Korea*
[2]*chemical engineering, Pohang University of Science and Technology, Korea*

For the emerging bio-compatible, wearable, and stretchable epidermal electronic devices, it is essential to realize novel stretchable conductors with the attributes of transparency, low-cost and non-toxic components, green-solvent processbility, self-healing, and thermal stabililty. Although conducting materials-rubber composites, ionic hydrogels, organogels were developed, no stretchable material system that could meet all the outlined requirements has been reported. Here, we design and synthesize a series of P(SPMA-r-MMA) polymers with different ratios of ionic side chain, and demonstrate for the first time that the resulting stretchable ionic conductors with glycerol are transparent, water processable, self-healable, and thermally stable due to the chemically linked ionic side chain, satisfying all aforementioned requirements. Among the series of polymer gels, the P(SPMA0.75-r-MMA0.25) gel showed optimum conductivity (6.7 x 10-4 S cm-1), stretchability (2636 % of break at elongation), and self-healing (98.3 % in 3 hours) properties. Accordingly, the transparent and self-healable P(SPMA0.75-r-MMA0.25) gels were used to realize thermally robust actuators up to 100 °C, and deformable and self-healable thermal sensors for the first time.

Oral Presentation : **POLY.O-3**
Oral Presentation for Young Polymer Scientists
Room 402 (Live Streaming) TUE 09:40
Chair: Seung Goo Lee (University of Ulsan)

Glutathione-sensitive peptide amphiphile vesicles designed for efficient drug transport controlled by positionable disulfide-bridges

Hayeon Kim, Eunji Lee*

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

In anti-cancer drug delivery systems, to deliver and release the loaded drugs to the target tumor cells is one of the major challenges due to systemic toxicity and the potential side effects on the normal cells. In this context, stimuli-responsive drug vehicles for controlled drug release, especially redox-sensitive nanoparticles have been developed. The vehicles based on the self-assembled peptide amphiphiles (PAs) are attracting attention for their dual loading capability for hydrophilic and hydrophobic payloads and biocompatibility. However, the controlled stability of the PAs vehicles in physiological media still remains a challenge for the efficient drug transport system. Here, the glutathione-adaptive vesicles that have drug loading/releasing capability were designed by self-assembly of PA containing thiol groups forming disulfide-linkage by the oxidation that can be cleaved in a reductive environment. The drug loading capacities and releasing efficiencies of PAs vesicles were investigated as functions of the position and number of disulfide-linkage during assembly. This research can provide a useful strategy to design biocompatible PAs vehicles for efficient drug-delivery and be a solid foundation for development of further nanocarrier for biomedical applications.

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

Oral Presentation for Young Polymer Scientists

Room 402 (Live Streaming) TUE 10:00

Chair: Seung Goo Lee (University of Ulsan)

Reversibly cross-linkable block copolymer for self-healing polymer materials to enhance thermomechanical property

Hyangmoo Lee, In Woo Cheong[1,*]

School of chemical engineering, Kyungpook National University, Korea
[1]*Department of Applied Chemistry, Kyungpook National University, Korea*

Damaging such as fractures and scratches cause deterioration of mechanical strength, toughness, surface gloss, and barrier properties, and it cause shortening of product life span. In this study, diblock copolymer was synthesized via reversible addition-fragmentation chain transfer (RAFT) polymerization with self-healable block (PtB) with bulky urea and hard-domain block (P4VP), and blended into PtB matrix polymer to form block copolymer micelles with various ratio in various solvents to form desired micellar structures, and the blends were cross-linked with hexamethylene diisocyanate (HDI). In this self-healing system, block copolymer micelles works as physical cross-linking points which can stand much higher temperature than cross-linking points formed by hindered urea. This feature can greatly expand the working temperature range of self-healing material. Prepared samples were analyzed by TEM, UTM, Rheometer, and others. This work was supported by the Ministry of Trade, Industry and Energy (No. 10067082) and the Ministry of Land, Infrastructure and Transport – South Korea (Grant No. 19POQW-B152733-01).

Oral Presentation : **POLY.O-5**
Oral Presentation for Young Polymer Scientists
Room 402 (Live Streaming) TUE 10:20
Chair: Seung Goo Lee (University of Ulsan)

Improving Solid-State Emission of Flat Aromatic Molecules by Edge-Functionalization with Picket-Fence Groups

Hye Jin Cho, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Polycyclic aromatic hydrocarbons (PAHs) are flat aromatic molecules composed of only carbon and hydrogen atoms. They are promising for material science, especially for light-emitting systems, optical sensors, photovoltaic cells, and organic field-effect transistors. The intrinsic properties based on their structure approved many advantages including high thermal and chemical stability, electron mobility, and unique photophysical characteristics. However, the rigid and flat structures of PAHs are like a double-edged sword that the strong π-π stacking forces them to aggregate, hence making them insoluble and difficult to handle. More significantly, stacked PAHs accompany severe undesirable changes in their photophysical properties, of solid-state in particular. Herein, we report a series of PAHs showing suppressed π-π stacking in both solution and solid-state via steric hindrance. A bulky 2,6-dimethylphenyl group, called “picket-fence (PF) group” in this study, was introduced on the edge of PAHs through bottom-up synthesis. It enabled PAHs to have excellent solid-state photophysical properties with significant enhancement in solubility. From experimental results combined with theoretical calculations, we found that the PF effect could be adjusted by the picket size. Finally we confirmed that our strategy using PF groups is effective enough to even large flat PAHs. We manufactured the first light-emitting device using HBC-based emitter, which the emission spectrum of the device exhibit single-molecular characteristic with the narrow full-width at half-maximum value of only 20 nm.

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

Oral Presentation for Young Physical Chemists

Room 403 (Live Streaming) TUE 09:00

Chair: Namdoo Kim (Kongju National University)

Modeling a Non-Electrochemical Reaction Electrochemically: DFT study of Hydrogen Peroxide Direct Synthesis on Palladium Surfaces

Min-Cheol Kim

Computational Science Research Center, Korea Institute of Science and Technology, Korea

The mechanism of catalytic non-electrochemical hydrogen peroxide direct synthesis (HPDS) from hydrogen and oxygen is conventionally considered as a Langmuir-Hinshelwood (LH) mechanism, i.e. (activated) H_2 and O_2 molecules react on the same site of a catalyst after adsorption. Conventional density functional theory (DFT) studies follows this assumption, simulating the reaction pathway of HPDS on catalyst surface with activated hydrogens forming a bond one-by-one with a activated O_2 molecule. A recent experimental study show that the conventional LH mechanism may not be true even on the most prototypical HPDS catalyst: palladium (Pd) catalysts. In fact, it is proposed that the "non-electrochemical" HPDS is actually a heterolytic redox reaction of H_2 and O_2 forming H_{2O2} with proton-electron transfer on Pd surfaces. In this presentation, we provide a DFT model for accurate descriptions of the reaction mechanism of HPDS on catalysts using the example of Pd 111 surface. We show that even with a more comprehensive model including solvation and free energy corrections, the LH mechanism fails to explain the experimental observations of HPDS. We then also attempt to model the hetrolytic mechanism by combining the Butler-Volmer equation with the electrochemical constant-potential DFT to compare the kinetics of the redox reaction with the LH mechanism, proving the redox reaction mechanism is indeed more feasible for Pd catalysts, and HPDS is kinetically favored than water production. Finally we discuss the limitations and possible improvements.

Oral Presentation : **PHYS.O-2**
Oral Presentation for Young Physical Chemists
Room 403 (Live Streaming) TUE 09:15
Chair: Namdoo Kim (Kongju National University)

Highly Efficient Single-Colloid Heat Engine with Active Noises

Taejin Kwon, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Since Feynman's visionary idea on tiny motors, constructing engines that operate at small scales has been one of the most challenging issues. The performance of microscale engines is influenced strongly by the surrounding environment because work extracted by the engines is of the same order of the energy fluctuation. A recent experiment realized a single colloidal heat engine in bacterial baths using optical a laser trap[1]. They showed that the efficiency of engines surpassed the equilibrium Carnot efficiency due to active noises. Despite the remarkable performance of active heat engines, it remains unclear how the active noise would lead to the enhanced efficiency of the engines. Here, we perform numerical simulations of the single colloidal heat engine with active noises. We find that the efficiency of the heat engine is sensitive to the interplay between the active noises and the relaxation dynamics of a trapped colloid particle. When the correlation time of active noises is much larger than the relaxation time of a trapped colloid particle, the efficiency of the active heat engine is about six times larger than that of heat engine without active noises. These results indicate that non-equilibrium effects by active noises increase the effective temperature of heat engines.[1] Sudeesh Krishnamurthy, Subho Ghosh, Dipankar Chatterji, Rajesh Ganapathy, and A. K. Sood, Nat. Phys. 12, 1134-1139 (2016)

Oral Presentation : **PHYS.O-3**
Oral Presentation for Young Physical Chemists
Room 403 (Live Streaming) TUE 09:30
Chair: Namdoo Kim (Kongju National University)

Polarized Raman Spectra and Complex Raman Tensors of Antiferromagnetic Semiconductor $CrPS_4$

Sujin Kim, Sunmin Ryu[*]

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

Chromium thiophosphate ($CrPS_4$), a monoclinic crystal of C^3_2 space group, is a ternary layered semiconductor with an optical bandgap of 1.4 eV and exhibits anti-ferromagnetism below 36 K. Despite its potential in optoelectronic and magnetic applications, the symmetry of its lattice vibrations has not been studied. In this work, we performed a polarized Raman spectroscopy of bulk $CrPS_4$ using three different excitation wavelengths of 457, 514 and 633 nm. High-quality crystals grown by the chemical vapor transport method were mechanically exfoliated or polished to expose three orthogonal crystallographic facets. Polarized Raman spectra were obtained in parallel and cross configurations by rotating samples about the surface normal to each of the facets. Among 33 Raman active modes (16 A and 17 B) at the Brillouin zone center, 19 (8) peaks observed in the parallel (cross) configuration were assigned as A (B) modes. Complex-valued Raman tensors were determined for 7 major A modes using the angle-dependent Raman spectra of the three facets. The results can also be used in determining crystallographic orientations of $CrPS_4$ unequivocally.(to be submitted)

Oral Presentation : **PHYS.O-4**
Oral Presentation for Young Physical Chemists
Room 403 (Live Streaming) TUE 09:45
Chair: Namdoo Kim (Kongju National University)

Replica ensemble enabled uncertainty estimation of neural network potentials with atomic-level resolution

Wonseok Jeong

Materials Science & Engineering, Seoul National University, Korea

Neural network potentials (NNPs) are gaining much attention as they enable fast atomic simulations for a wide range of systems while maintaining the accuracy of density functional theory calculations. Since NNP is constructed by machine learning on training data, its prediction uncertainty increases drastically as atomic environments deviate from training points. Therefore, it is essential to monitor the uncertainty level during the simulations to judge the soundness of the results. In this presentation, we present an uncertainty estimator based on the replica ensemble in which NNPs are trained over atomic energies of a reference NNP that drives the target simulations. The replica ensemble is trained efficiently and its standard deviation provides atomic-resolution uncertainties. We apply this method to a silicidation process of Ni deposited on Si(001) and confirm that the replica ensemble can spatially and temporally trace simulation errors at the atomic resolution, which in turn guides on augmenting the training set. The refined NNP completes a 3.6-ns molecular dynamics simulation without any noticeable defects. The efficient and atomic-resolution uncertainty indicator suggested in this presentation will contribute to achieving reliable NNP simulations.

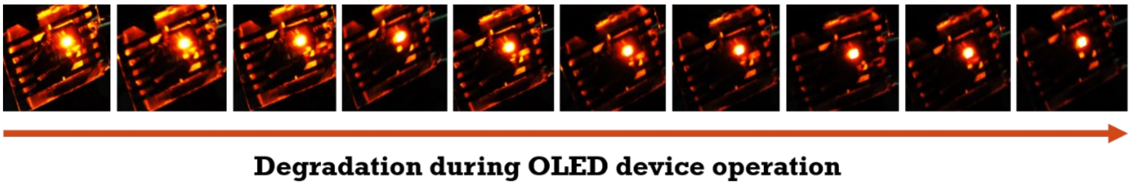
Oral Presentation : **PHYS.O-5**
Oral Presentation for Young Physical Chemists
Room 403 (Live Streaming) TUE 10:00
Chair: Namdoo Kim (Kongju National University)

Discrimination of Degradation Mechanism for OLED by Noninvasive, Layer-selective Analysis

Jung Bae Son, Seong Keun Kim[*]

Division of Chemistry, Seoul National University, Korea

Despite the importance of elucidating the degradation mechanism of the organic light-emitting diodes (OLEDs) and the role of each layer played in degradation, little is known to date. To gain an insight into the cause of degradation and decouple the effects of different layers on degradation, we devised a method for layer-selective analysis of OLED devices. We fabricated OLED panels with 3 layers (each for electron transport, emission, and hole transport) whose emission wavelengths and lifetime are distinct from one another, and thus can be discriminated against each other. We found two types of degradation mechanism and different degradation features for each layer. These results raise the prospect of understanding the ultimate cause of degradation by noninvasively tracking the whole layers during actual operation. In addition, the method we developed here can be readily adopted in other studies as a powerful diagnostic tool for improving device characteristics.



Oral Presentation : **PHYS.O-6**
Oral Presentation for Young Physical Chemists
Room 403 (Live Streaming) TUE 10:15
Chair: Namdoo Kim (Kongju National University)

Development of Ultra-low Frequency ($^{-1}$) Raman Spectroscopy and Studies of Absolute Raman Cross-sections of Sulfur Film

Mingyeong Shin, Juwon Kim, Yeonsu Jeong, Myeongkee Park[1,*]

Chemistry, Dong-A University, Korea
[1]*Department of Chemistry, Dong-A University, Korea*

Recently, the diverse scope of ultra-low frequency Raman studies has greatly grown because interlayer and skeletal vibrations are located at $^{-1}$ correlated to specific interactions of functional materials, such as graphene, WS_2, and perovskites. However, quantitative analyses using absolute Raman cross-sections (σ_R) have less studied than qualitative analyses using normalized Raman spectra. σ_R is the effective area proportional to the possibility of Raman scattering by an incident excitation. This σ_R can be determined by Equation 1. F is the integrated area under the photon flux for Raman mode. P_p is the pump power incident upon the sample. N is the atomic concentration of sulfur and L is the effective thickness that contributes to scattering. h_{vp} is the photon pump energy. η_c is the optical collection efficiency of Raman spectrometer. We have developed a home-built ultra-low frequency Raman spectrometer and measured σ_R of sulfur at $^{-1}$. (Figure 1) In this talk, we will present our on- and off-resonant absolute σ_R values of sulfur. We expect these σ_R of sulfur can be the relative references for quantitative ultra-low frequency Raman studies of materials.

$$\boldsymbol{\sigma_R = \frac{Fh_{vp}}{\eta_c P_p N L}} \qquad \textbf{Equation(1)}$$

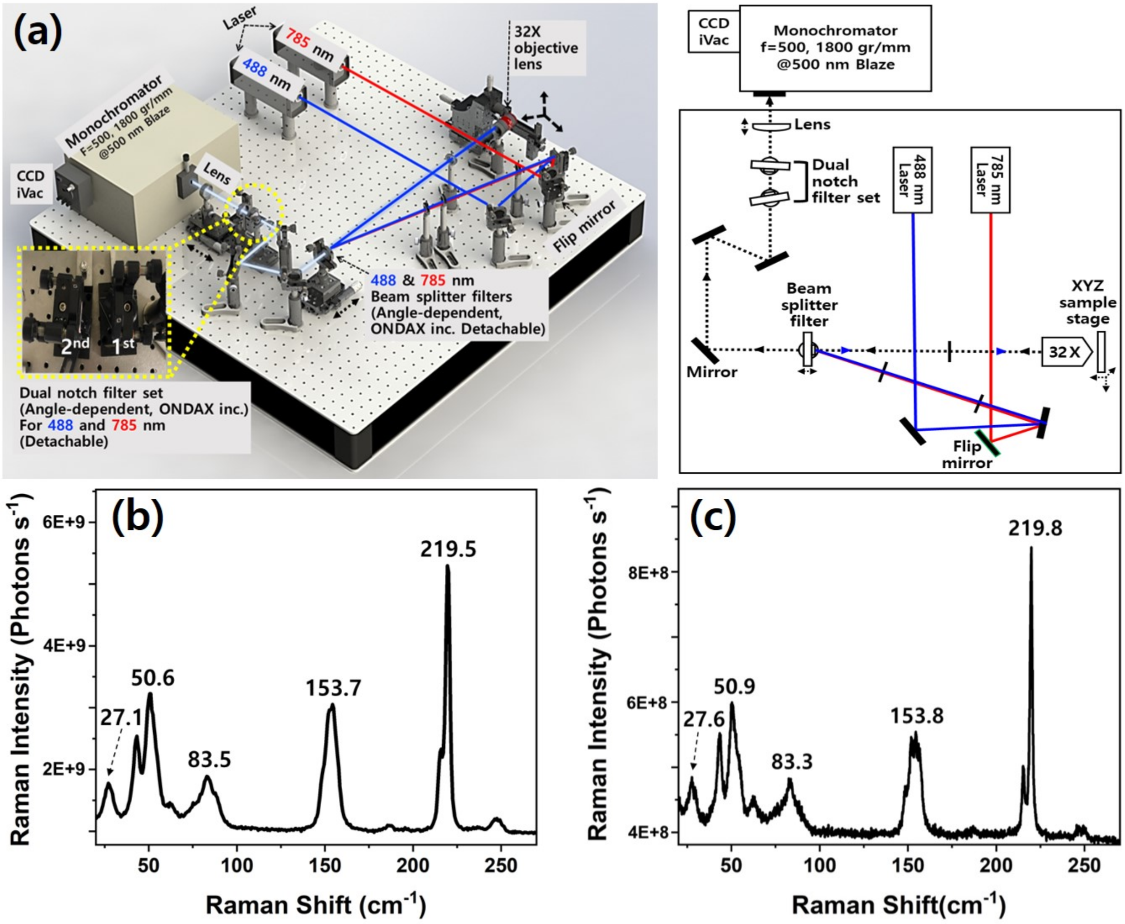


Figure 1. (a) Schematic of the Home-built Raman spectrometer for ultra-low frequency detections and Raman spectra of 35-μm-thick polycrystalline sulfur film excited at (b) 488 and (b) 785 nm.

Oral Presentation : **ANAL1.O-1**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:00
Chair: Young-Kwan Kim (Dongguk University)

All electronic, single-molecule bioassay by carbon-nanotube field effect transistor arrays

Yoonhee Lee, Kenneth L. Shepard[1,*]

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

[1]*Department of Electrical Engineering, Columbia University, New York, US, United States*

Field-effect transistors (FETs) allow label-free detection of molecules by transducing the intrinsic charge of molecules into the device's conductance. Considerable effort has been directed to the development of field-effect-transistor-based biosensors, in which detection is based on the charge of an ensemble of captured molecules gating the current in a transistor. The read-out in these devices is the amplitude of the drain current, a signal that is unfortunately easily corrupted by nonspecific interactions with other charged molecules. Here, we demonstrate how a new class of sensors, the single-molecule field-effect transistor (smFET), can detect the charge on a single molecule and be used for bioassay. For genomic assays, detection is achieved with a single-stranded DNA (ssDNA) probe molecule, tethered on the SWCNT. We develop a point-functionalization method for the single-probe attachment that is electrically controllable and applicable to many devices in parallel in arrays. In each device, DNA hybridization events are encoded temporally, and their kinetics are modulated by biasing the surrounding electrolyte relative to the device. This electronic bioassay system expands the utility with other probe molecules. For example, an aptamer probe on a device allows neurotransmitter sensing by monitoring dynamic conformational change associated with small-molecule binding to the aptamer structure.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:04

Chair: Young-Kwan Kim (Dongguk University)

Effective determination of chiral nicotine using Dispersive Liquid-Liquid Microextraction HPLC/UV-vis

Seung Hoon Song, Seung Woon Myung*

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Nicotine is a stimulant and powerful alkaloid, usually derived from tobacco plants, but this nicotine can also be obtained through chemical synthesis. In the case of natural nicotine, the content of (S)-nicotine is overwhelmingly higher than that of (R)-nicotine. Synthetic nicotine is mainly used for e-liquid production. In this study, we performed an improvement of the nicotine extraction method using DLLEME to differentiate between natural nicotine and synthetic nicotine and to effectively separate chiral nicotine. In order to optimally extract nicotine from each sample, the sample using high performance liquid chromatography (HPLC) / UV-Vis after comparing the type of dispersion solvent, pH, and amount of salt that can be used in DLLME to obtain optimal efficiency. optimally Established a method to separate and quantify chiral nicotine.. Experiments were conducted to confirm the matrix effect and to determine the optimal solvent conditions. Chromatographic separation using HPLC/UV-Vis was performed using a CHIRALCEL OD-H (4.6 mm id x 250 mm length, 5 μm particle size) column and isocratic conditions with hexane and ethanol. By using this method, chiral nicotine present in the sample is extracted more efficiently, enabling quantitative and qualitative analysis.

Oral Presentation : **ANAL1.O-3**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:08
Chair: Young-Kwan Kim (Dongguk University)

Flow field-flow fractionation with thickness tapered channel

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Flow field-flow fractionation (FlFFF) is a separation method that is capable of fractionating particulate or macromolecules by the differences in the hydrodynamic diameters of sample components in an empty channel space. FlFFF utilizes two perpendicular flow streams: migration flow to drive sample components to migrate along the channel and crossflow to retain sample materials within the channel. In general, separation is achieved by the increasing order of diameter typically in the normal operating mode and it useful to separate biological macromolecules or particles with broad molecular weight or diameter distribution. While separation efficiency in FlFFF increases with the increase of channel thickness, it increases the separation time and often induces poor recovery of long retaining components such as large MW or diameter species. To overcome this issue, FFF has been commonly utilized with field programming method in which the field strength gradually decreases with time so that retention time can be shortened with the increase of sample recovery and resolution. However, additional hardware to control the two flow rates is required for the programming of the field strength in FlFFF. In this study, a new type of channel with tapered thickness for asymmetrical flow field-flow fractionation is introduced. Thickness tapered channel exhibits a field programming effect without any software or instrument owing to the increasing migration flow velocity along the channel axis. Separation efficiency of the thickness tapered channel was investigated in various flow rate conditions by comparing retention time, peak width, and peak height to those of the channel with uniform thickness.

Oral Presentation : **ANAL1.O-4**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:12
Chair: Young-Kwan Kim (Dongguk University)

Effect of reduced Graphene oxide and $MnFe_2O_4$ nanoparticles on Carbonyl Iron for Magnetorheological Fluids

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Magnetorheological(MR) fluids are colloidal suspensions of magnetic particles dispersed in non-magnetic liquid medium such as silicone oil. They change from a fluid-like to a solid-like structure under an external magnetic field, resulting in a significant increase in shear viscosity, yield stress, and dynamic modulus. Carbonyl iron(CI) particles have been used as magnetic materials for MR fluids due to their proper particle size and high saturation magnetization, but they cause serious sedimentation problems in MR fluids. To solve this problem, two different kinds of additives were introduced to the CI solution in this study. Graphene oxide(GO) is expected to improve the dispersion and sedimentation stability of MR fluids due to its low density, planar structure and large specific surface area. $MnFe_2O_4$ is also expected to improve distributed stability and magnetorheological characteristics because it has high magnetization rate, low density and distinct magnetism. The aqueous CI solution was first mixed and sonicated with sodium hydroxide and GO, and then transition metal solutions of manganese(II) nitrate and iron(III) chloride was slowly added to the CI solution, preparing in CI/ $MnFe_2O_4$/GO. The final product, CI/ $MnFe_2O_4$/rGO, was synthesized by annealing to reduce GO to rGO. The CI/$MnFe_2O_4$/rGO was dispersed to the silicon oil by ultrasonication. The morphologies, compositions and crystal qualities of the prepared CI/$MnFe_2O_4$/rGO composites were characterized by SEM, EDS, TEM, XRD and XPS. The magnetic properties of CI/$MnFe_2O_4$/rGO were measured using a VMS. The MR performances of the prepared MR fluids were investigated by a rotating rheometer.

Oral Presentation : **ANAL1.O-5**

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:16

Chair: Young-Kwan Kim (Dongguk University)

SERS-based immunoassay of thyroid-stimulating hormone (TSH) using silver-encapsulated gold nanoparticles and fabrication of 3D paper fluidic chips

Kyeongnyeon Kim, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

Thyroid-stimulating hormone (TSH) is essential for regulating the body`s metabolism and is also used as a biomarker for the diagnosis of hyperthyroidism (inhibited) and hypothyroidism (elevated). Lateral flow assay (LFA) strips can be used for the diagnosis of hypothyroidism but there is no commercially available one for hyperthyroidism since it is difficult to detect an extremely low TSH concentration in human serum. Radioimmunoassay (RIA), immunochemiluminescent assay (ICMA) and enzyme-linked immunosorbent assay (ELISA) methods are used to detect TSH below the normal range from 0.5 to 5 uIU/mL but they have several drawbacks including a long assay time and high cost. Herein, we report the fabrication of a conceptually new 3D paper fluidic chip and the production of silver-encapsulated Au nanoparticles (Ag-AuNPs) for highly sensitive detection of TSH. Ag-AuNPs generate hot spots at the nanogaps between Ag shell and Au core, and consequently induce a greatly enhanced Raman signals. It is possible to diagnose hyperthyroidism as well as hypothyroidism since a TSH concentration lower than 0.5 uIU/mL can be detected using these techniques. We believe that this approach can be also used for the diagnosis of other hormones that require high sensitivity.

Oral Presentation : **ANAL1.O-6**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:20
Chair: Young-Kwan Kim (Dongguk University)

SERS-PCR assays of SARS-CoV-2 using three-dimensional plasmonic nanodimple substrates.

Yixuan Wu, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

As evident from the ongoing COVID-19 pandemic, a rapid and accurate diagnosis of infectious diseases is crucial for effective prevention of disease spread. Real-time polymerase chain reaction (RT-PCR) technique is considered as a current gold standard for diagnosis of SARS-CoV-2. Fluorescence detection method using TaqMan probes is used for the detection of terget genes after 30-40 thermocycling steps in RT-PCR. However, it often lacks the detection sensitivity for rapid and accurate detection of terget genes. Therefore, it is important to develop a sensitive detection method to reduce the time for diagnosis of SARS-CoV-2. Herein, we report a surface-enhanced Raman scattering based polymerase chain reaction (SERS-PCR) assay platform for the rapid detection of SARS-CoV-2. To enhance the Raman signals, three-dimensional nano-dimple plasmonic substrates were employed as a SERS assay platform. It was possible to detect the target gene at 32 copies/μL level after 20 PCR cycles by the SERS-PCR, while it takes approximately 40 PCR cycles to detect a target gene by RT-PCR. Thus, this SERS-PCR demonstrates a strong potential to be used as a rapid detection method for diagnosis of SARS-CoV-2.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:24

Chair: Young-Kwan Kim (Dongguk University)

Identification of cervicovaginal fluid metabolites associated with preterm birth

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Preterm birth (PTB) is defined as fetal birth less than 37 weeks of pregnancy, and is a serious problem of the neonate and maternal health with the risk of mortality and morbidity. During pregnancy, there are physiological changes, such as the interaction between the maternal microbiota and the fetus environment, which affect the composition of the vaginal microbial cluster. To date, very limited studies are available that have examined the putative microbiota metabolites for preterm birth. Thus, it is necessary to find specific biomarkers that can predict preterm birth for an in-depth understanding of the vaginal microbiota metabolites inducing preterm birth. In this study, we analysed vaginal microbiota metabolites to identify markers that can predict preterm birth compared to term birth. We performed metabolic profiling using nuclear magnetic resonance (NMR) spectroscopy to investigate metabolites in cervicovaginal fluid (CVF) samples from pregnant women with preterm birth and term birth. The 8 metabolites were significantly increased in the preterm birth group compared with the term birth group, and these metabolites could be beneficial markers for clinical application of preterm birth predictions.This study demonstrates certain CVF metabolites have shown significant changes in the preterm birth compared to term birth and metabolomics approach can be used to investigate markers predicting preterm births.

Oral Presentation : **ANAL1.O-8**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:28
Chair: Young-Kwan Kim (Dongguk University)

An Untargeted Analysis of Metabolite Biomarkers in Urine for Miscarriage/Pre-term Birth using LC-MS/MS

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Miscarriage is a birth-related issue that carries a pregnancy loss before 20 gestational weeks of pregnant women. According to Ministry of Health and Welfare of Korea, the rate of preterm birth in Korea has increased double in 2017 compared to the rate in 2000. There have been different approaches to find possible biomarker candidates, like proteins and lipids, related to miscarriage in urine, serum and plasma of pregnant women. However, no biomarker candidates related to preterm birth or miscarriage were identified, and more comprehensive search for the possible biomarker is required for metabolites and metabolic by-products.In this study, a dansyl reaction was utilized to search for metabolic biomarkers, which derivatizes various metabolites in urinary sample from pregnant women and patients experienced miscarriage. In the dansyl reaction, metabolites and metabolic by-products with amines and phenol functional groups could be derivatized using dansyl chloride and those with carbonyls and carboxyl functional groups could be labeled with dansyl hydrazine. We plan to identify and quantify derivatized metabolites in urinary samples using liquid chromatography tandem mass spectrometry (LC-MS/MS). Also, other metabolites like lysine, tyrosine and citrate were analyzed quantitatively as well. A deuterated internal standard for each metabolite was spiked into each urine sample and creatinine were also analyzed to precisely quantitate the metabolites in each urine samples. This research was supported by the Ministry of Health and Welfare of Korea (HI17C1238).

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:32

Chair: Young-Kwan Kim (Dongguk University)

Synthesis and structural studies of $LiFe_{1-x}Mn_xBO_3$ and $LiFe_{1-x}Co_xBO_3$ as a cathode material for Li–ion battery

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Successful operation of secondary Li-ion battery (LIB) relies on high-performance cathode materials that control the cost and energy density. Thus, battery community has been focused on discovery and development of cathode materials. These days, the cathode materials can be divided into two categories: lithium metal oxide and polyanionic compounds. Polyanionic structure compounds are widely studied as a cathode material for LIB. Among them, lithium metal borate ($LiMBO_3$, M= Mn, Fe or Co) forms have the lowest weight, thus offering the highest theoretical capacity (220 $mAhg^{-1}$). Also, the energy density is expected to be higher than phosphates. Among borate based materials, $LiMnBO_3$ has high operating potential, while $LiFeBO_3$ has high theoretical capacity. And $LiCoBO_3$ has the excellent combination of high theoretical capacity (215 $mAhg^{-1}$) and expected 4 V operation. Therefore, $LiFe_{1-x}Mn_xBO_3$ and $LiFe_{1-x}Co_xBO_3$ (x = 0, 0.25, 0.5, 0.75, and 1.0) composite materials have been synthesized with solid-state reaction method for structural studies according to the amount of electrons on metal sites. The morphology and structural studies of synthesized materials have been identified X-ray diffraction (XRD) and ^{7}Li MAS NMR. Also, quantitative analysis for the ratio of Mn : Fe and Fe : Co has been performed with laser induced breakdown spectroscopy (LIBS).

Oral Presentation : **ANAL1.O-10**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:36
Chair: Young-Kwan Kim (Dongguk University)

Synthesis and Electrochemical Properties of Sulfate-based Yavapaiite-like Structure for Promising Polyanionic Cathode Material

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Department of Chemistry, University of Ulsan, Korea

Domination of lithium-ion batteries (LIBs) have become sophisticated for electrical energy storage technology. However, depending on their applications, development of new electrode materials for LIBs especially with polyanionic compound needs to fulfill aspects such as high gravimetric and volumetric energy density, low-cost, charge/discharge rate, safety issues, and term of sustainability. Despite of $LiFePO_4$ as well-known cathode material, $Li_2V_2(SO_4)_3$ and $Li_2VO(SO_4)_2$ are shown good evidence of inductive effect for polyanionic material such as borate, phosphate, and silicate. In this study, novel lithium vanadium sulfate-based polyanionic cathode material via low temperature eco-efficient solution method has been developed. Electrochemical reversibility of active material has been conducted by 2016-coin cell with range of operating voltage 3.0 V – 4.8 V. X-ray diffraction pattern and infrared spectra support structural characterization of the material. Electrochemical performance of the first discharge has been obtained 36.45 mAh/g with C/20 rate. High potential of 3.85 V to extract Li-ion and charge voltage of 4.3 V for re-insertion process have been used.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:40

Chair: Young-Kwan Kim (Dongguk University)

Kinetic modulation of Amyloid-β through its point mutation by structure-based design

Dongjoon Im, Chae Eun Heo, MyungKook Son, Chae Ri Park, Sooyeon Chae, Min Ji Kim[1], Hugh I. Kim[*]

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Modulating the formation process of amyloid-β fibril, especially kinetically delaying its early onset, is an applicable solution for Alzheimer's disease patients along with early diagnosis. The aggregates of Amyloid-β (Aβ) fibrils which are commonly observed in the brain of the Alzheimer's disease patients are considered to be closely related to the pathogenesis of the disease. Amyloid-β peptides with different number of residues may look alike but clearly have different physical properties. The peptides consisting of 40 and 42 amino acids, the two most dominant species, only differ in two amino acids of the N-terminal which is what provokes the difference of the entire morphology of their fibril structure, accelerated fibrillation of Aβ 42 to Aβ 40 as well as other properties. Since Aβ 42 to Aβ 40 ratio is found to be higher in patients compared to non-patients, we suggested the distinct physical properties of Aβ 42 to act as key factors in making it prone to self-assembly. In this study, we rationally designed mutant peptides with various point mutations based on their structure and physical properties. Designed mutant peptides have not only shown suppressed self-assembly, but also slowed down fibrillation process when mixed with wild type Amyloid-β (1-42).

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:44

Chair: Young-Kwan Kim (Dongguk University)

Influence of the Preferred Orientation of Pyridine Derivatives with Donor Substituents on Chemical Interface Damping Induced in Silver-Coated Gold Nanorods with Different Shell Thicknesses

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Chemical interface damping (CID) is one of the plasmon decay processes caused by adsorbate molecules in gold nanoparticles. Despite the advances in this field, the effect of pyridine derivatives having a preferred orientation on CID in silver-coated gold nanorods (AuNRs@Ag, core@shell) with different shell thicknesses remains unknown. Herein, dark-field scattering studies using pyridine derivatives with donor substituents as adsorbates in single AuNRs@Ag with two different Ag shell thicknesses are described. Pyridine derivatives having electrondonating groups (EDGs) were adsorbed on single AuNRs@Ag and induced a strong CID through the interaction of nitrogen with the Ag surface. AuNRs@Ag with thick shells showed a considerably enhanced CID effect compared with AuNRs@Ag with thin shells for all pyridine derivatives. Furthermore, pyridine derivatives with EDGs in the para position (4-aminopyridine and 4-dimethylaminopyridine) caused a decrease in the localized surface plasmon resonance (LSPR) linewidth broadening of single AuNRs@Ag compared with unsubstituted pyridine under the same experimental conditions. In contrast to the high inclination of pyridine molecules, pyridine derivatives bearing EDGs adopted a parallel orientation to the Ag surface according to surface-enhanced Raman spectroscopy and dynamic light scattering measurements, which resulted in different surface coverage on the Ag surface and decreased LSPR linewidth broadening. Therefore, this study provides deeper understanding of the effects of pyridine derivatives with donor substituents and Ag shell thickness on CID in single AuNRs@Ag.

Oral Presentation : **ANAL1.O-13**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:48
Chair: Young-Kwan Kim (Dongguk University)

Tunable Chirality in Two Thumbs film

Juyong Gwak

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Nature-mimmetic chiroptical metasurface has become a challenging flat optics research theme to apply stereochemistry, molecular biology, crystallography, and further secure quantum communications. In this article, chiral metasurfaces transferred from commercial optical grating were fabricated by using a polydimethylsiloxane (PDMS) film, in which the chirality of the metasurface film was readily tuned to be left- and right-handed by modulating the angle (θ) between the curvature vector and the grating direction, i.e., blaze arrow. Furthermore, a fingerprint – transferred PDMS metasurface with Au coating was prepared to investigate nature-induced chirality and surface plasmon resonance (SPR). Indeed, the fingerprint-transferred metasurface showed unique chiroptical SPR property, induing surface enhanced Raman scattering (SERS) effect to monitor chiral molecules. It is probably ascribed to the grating-like pattern and curvature of the PDMS film transferred the human thumb, similar to the as-designed grating. It is probable that these results will open a novel approach to produce facile chiral metasurfaces.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) TUE 09:52

Chair: Young-Kwan Kim (Dongguk University)

Comparison of Fibrillation Kinetics of Amyloid Proteins in H2O and D2O

MyungKook Son, Chae Ri Park, Chae Eun Heo, Dongjoon Im, Min Ji Kim, Sooyeon Chae, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Heavy water, D2O, has been used in Infra-Red (IR) spectroscopy, Nuclear Magnetic Resonance (NMR), etc., to avoid the interference of O-H frequencies and H resonance frequency when light water, H2O is used. Specifically for IR, amide I band of peptides and proteins is 1600-1700 cm-1, while the H2O vibrational frequency is 1643.5 cm-1 overlapping the amide I band. Also, hydrogen-deuterium exchange (HDX) mass spectrometry is utilized to study protein tertiary structures.But since D2O is more polar than that of H2O, the hydrophobic effect of D2O is also stronger. So, the properties of the protein in H2O and D2O for example, protein stability, can be different. Efimova et al., have compared the stability of globular protein, lysozyme and bovine serum albumin in H2O and D2O, using differential scanning calorimetry (DSC). Proteins were more stable in D2O, with a wider pH range of stable form of BSA. There are some similar studies, but little about the protein fibrillation in D2O is known. Hydrophobic interaction of proteins is significant to the fibrillation of amyloidogenic proteins and protein structures. In this study, we have compared the hydrophobic interactions, structures and stability of amyloidogenic proteins, insulin and alpha-synuclein, using various spectroscopic methods, Fourier transform IR (FT-IR) spectroscopy, 2D-IR spectroscopy, ion mobility mass spectrometry, small angle x-ray scattering, thioflavin-T assay, DSC, etc.

Oral Presentation : **ANAL1.O-15**
Oral Presentation of Young Analytical Chemists I
Room 301 (Live Streaming) TUE 09:56
Chair: Young-Kwan Kim (Dongguk University)

Photothermal effect analysis of Bi-Te covered nanorods on 3D spheroid neuroblastoma cells

Chae ri Park, Chae Eun Heo, MyungKook Son, Dongjoon Im, Min Ji Kim, Sooyeon Chae, Hugh I. Kim[*]

Department of Chemistry, Korea University, Korea

Neuroblastoma is a solid tumor that almost always affects children. It starts in immature nerve cells found in an embryo or fetus. These days, nanoparticle for cancer treatment is being actively studied. The major function of these nanoparticles in therapy is drug delivery vesicles, imaging agents, and photothermal effect etc. So far, most studies of nanoparticle have been based on two-dimensional (2D) cell models. However, 2D cell models are hard to provide an accurate representation of the in vivo environment of the solid tumor. In this study, we use three-dimensional (3D) human neuroblastoma SK-N-SH cell spheroid models instead of 2D cell models to overcome the limitation of 2D cell models. After 5 days of culturing 3D spheroids, we treated Bi-Te covered nanorods (BTCN) that is previously reported for its photothermal and photoacoustic effect on 2D cancer cell models. BTCN is dissolved in serum free media and treated at spheroids with various concentrations for 4 hours. Then, 808nm 5 W/cm2 near IR laser light is irradiated for 2 minutes per one spheroid. After this process, we measured cell viability of the spheroids to identify the effect of BTCN with laser irradiation in 3D cell models. Also, we examine a form of the spheroids through a microscope, looked at the distribution of living cells and dead cells through confocal microscope. The results obtained from these techniques will help us to find out the difference between the therapeutic effects of BTCN in the 2D and 3D cell models, and how to increase their effectiveness in 3D cell models that is similar to reality.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) TUE 10:00

Chair: Jongcheol Seo (POSTECH)

Amplification-free detection of COVID-19 target genes using a SERS-based microdroplet chip

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The coronavirus disease 2019 (COVID-19) outbreak has been labelled an ongoing pandemic by the World Health Organization (WHO). Real time quantitative polymerase chain reaction (RT-qPCR) has been recently considered a gold standard for the quantitative evaluation of a target gene but it still suffers from the problem of a long thermocycling time. To address this issue, we developed a surface-enhanced Raman scattering (SERS)-based DNA detection platform for the rapid and sensitive detection of target DNA markers of corona virus. Just like the RT-qPCR, two DNA probes, a broad-range probe for E gene and an additional probe for RdRp gene, have been used for the simultanelous detection two target DNAs of corona virus. The Raman signals of DNA markers were measured under flowing conditions. Total analysis time from droplet generation to SERS detection takes less than 10 min because all experimental conditions are automatically controlled inside the exquisitely designed microfluidic channel. This novel SERS-based DNA sensing technology in a microdroplet channel is expected to be a powerful analytical tool to simultaneously detect multiple DNA oligomer markers of infectious disease.

Oral Presentation : **ANAL2.O-2**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:04
Chair: Jongcheol Seo (POSTECH)

Size sorting of extracellular vesicles from cell using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

Young Beom Kim, Myeong Hee Moon[*]

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Extracellular vesicles (EVs) are cell-derived membrane-covered particles containing proteins, lipids, nucleic acids and other biological molecules. EVs play an essential role in the communication between cells via transporting pathologically important molecules. As the pathological importance of EVs increases, the expectation of EVs as a biomarker is growing. Subpopulations of EVs are divided into exosomes (30-100 nm in diameter) and microvesicles (100-1000 nm) according to their sizes and therefore, it is important to separate them because they differ in cellular origins, contents, and lipid compositions. However, it is challenging to isolate EVs while each of the separation methods such as ultracentrifugation, size exclusion chromatography, filtration, and precipitation has its own limitation.Field-flow fractionation (FFF) is a separation method capable of fractionating particles from nano to micron size in aqueous solution without using packing materials. In this study, exosomes and microvesicles secreted from cells were separated by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) with field programming and monitored by UV and multi-angle light scattering (MALS) detectors. Eluted exosomes and microvesicles were identified by western blotting and their sizes were determined by MALS and dynamic light scattering (DLS). Further, 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.

Oral Presentation : **ANAL2.O-3**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:08
Chair: Jongcheol Seo (POSTECH)

Microfluidic analytical device for Nucleic Acids Amplification and Detection

Nguyet mai Ly, Veasna Soum, Nayoon Pyun, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Polymerase chain reaction (PCR) for nucleic acid amplification plays an important role in genetics study as well as practical applications in diagnosis and detection, quality control, and quantitative monitoring of diseases, pathogens, or potential biomarkers. Conventional PCR is limited by time, equipment, tools, and skills of technicians. Many research groups have aimed to miniaturize PCR into a lab-on-chip device for point-of-care testing (POCT). Traditional approach is to use heating blocks with microfluidic device on which the flow is controlled by a supportive pumping system. To avoid dependence on pump, here we plan to build up a pumpless PCR chip controlled by capillary flow for self-regulated liquid delivery. Additionally, the flexible printed heaters on polyimide film fabricated by inkjet printer using conductive nano-silver ink have been provided for the underneath heating bed. For simple detection and easy visualization of amplified PCR products, a lateral flow assay will be employed later. This comprehensive device will promise a portable platform for POCT, being capable to complete both amplification and detection of target nucleic acid.

Oral Presentation : **ANAL2.O-4**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:12
Chair: Jongcheol Seo (POSTECH)

Synthesis and application of CNFs/GQD/SiNPs and CNT/GQD/SiNPs composites as anodes for Lithium-ion batteries

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[1]*Department of Applied Chemistry, Andong National University, Korea*

We used graphene quantum dots instead of graphite, which is one of the most popular anode material for existing lithium ion batteries. Silicon nanoparticles (SiNPs) and carbon nanomaterials are introduced to synthesize carbon nanofibers/graphene quantum dots/silicon nanoparticles (CNFs/GQD/SiNPs) and carbon nanotubes/graphene quantum dots/silicon nanoparticles (CNT/GQD/SiNPs) composites to improve their low capacity of carbon materials. To fabricate these composites, we positively charged SiNPs by adding poly(diallyldimethylammonium chloride)(PDDA). Subsequently, we combined the positively charged SiNPs with OH-GQDs using electrostatic attraction followed by mixing and dispersing the GQD/SiNPs nanocomposites with CNFs and CNT, respectively. After stirring, we filtered and dried the composites in the oven. The composites are reduced through annealing under Ar/H2 gases. The finally produced material is assembled into a coin cell to test battery performance which undergoes CV, rate capability, cycling test, and EIS. Before blending carbon nanomaterials, the discharge capacity of GQD/SiNPs composites is approximately 811.8mAh/g after 100 cycles. In addition, the prepared materials are characterized to investigate their physical properties via SEM/EDS, TEM, XRD, XPS, Raman, and FT-IR. We expect that these composites not only increase charging capacity, but also enhance the overall performance of the batteries by complementing each components' shortcomings.

Oral Presentation : **ANAL2.O-5**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:16
Chair: Jongcheol Seo (POSTECH)

Synthesis of Red Luminescence Carbon dot by Eu^{3+} and Detect Method

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Carbon quantum dot (CQD) is a new class of Carbon based fluorescent nano materials (less than 10nm in size), which has recently attracted considerable attention due to their superior properties of stability, bio-compatibility, low toxicity, good water solubility. The luminescent properties of CQD depend on the funtional groups contained on their surfaces. The lanthanide based luminescent nano structures have been recognized for their better chemical and optical properties originating from their electronic structures of *f*-orbital electrons. Europium has red luminescent fluorescence and sharp peak characteristic at 615nm($^5D_0 \rightarrow {}^7F_2$) of line type red *f*-*f* emission. Research for Eu^{3+}-modified CQD has been actively pursued because it is soluble in water and has a wide range of applications : light-emitting diode, organic lgith-emitting diode, bioimaging, sensing and targeting specific DNA structures.In during of CQD synthesis, we tried to combine Eu but the Eu^{3+} emission is rapidly quenched by water for OH^-. Several papers have found that using β-diketone caused complexing with Eu and could prevent Eu from losing a red light. When composing CQD, Eu was added, β-diketone was used to block OH^- ions, and the red light from Eu-CQD under UV lamps was finally determined. Also the width peak under UV lamps was measured at a rapid peak of λ_{em}=615nm in the expiratory spectrum. By introducing this method, the carbon dots that combine Europium are expected to be used in various filed today.

Oral Presentation : **ANAL2.O-6**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:20
Chair: Jongcheol Seo (POSTECH)

Method Validation of N-nitrosodimethylamine in Diltiazem by UPLC-ESI-SRM/MS

Keewon Yang, Jae-ung Lee[1], Han Bin Oh[1,*]

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In 2018, N-nitrosodimethylamine (NDMA) was first found in Valsartan, which is a drug used for treating hypertension. Since then, NDMA has been discovered in other drugs like Ranitidine and Metaformine. International Agency for Research on Cancer (IARC) classified NDMA as ‘2A’ type chemical, which is a chemical that may act as a carcinogen over ingestion. Different approaches, like GC-MS/MS, thermal desorption GC-MS and LC-MS/MS, were used to identify and quantify NDMA in different drugs and products. In this study, a method validation on NDMA in Diltiazem using the UPLC-ESI-SRM/MS was carried out to see if the method satisfies the guideline suggested by the KP/ICH and Ministry of Food and Drug Safety. Different criteria, like system suitability, specificity, linearity, accuracy, precision, limit of detection (LOD), limit of quantitation (LOQ) and robustness, were verified. Specificity of NDMA was tested for standard solutions prepared in methanol and two different matrices, capsule and tablets, which turned out to be no difference between the matrices. LOD and LOQ for NDMA in standard solution were 0.1 ng/mL and 2 ng/mL, respectively. The correlation coefficient (R2) of the linear regression line obtained in the concentration range of 2–100 ng/mL was 0.9992. The accuracy and precision of the method were also satisfied. In the future study, inter-laboratory precision and robustness of the method will be verified for drug substances and drug products.This research was supported by Ministry of Food and Drug Safety (20173MFDS162).

Oral Presentation : **ANAL2.O-7**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:24
Chair: Jongcheol Seo (POSTECH)

Serum metabolic profiling in morbid obese patients after bariatric surgery using NMR and LC/MS

Yeyoung Han, Do Hyun Ryu[1,*], Geum-Sook Hwang[*]

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Bariatric surgery is one of the most effective treatments for obesity and its complications. However, metabolic changes in bariatric surgery are not clear. In this study, we performed metabolic profiling of serum from 38 morbid obese patients who underwent bariatric surgery using nuclear magnetic resonance spectroscopy (NMR) and liquid chromatography/ mass spectrometry (LC/MS). We integrated metabolic profiling and gut microbiota profiling data to observe changes in human metabolism and intestinal environment after bariatric surgery. Samples were collected before surgery and 6 months after surgery. In global profiling using NMR, metabolites including amino acids, organic acids, carbohydrates, and short chain fatty acids were identified in serum of patients. Principal component analysis (PCA) score plot showed a clear separation between before surgery and after surgery group. We found that serum metabolites associated with obesity metabolism (branched-chain amino acids (BCAAs) and aromatic amino acids) and metabolites related to energy metabolism (glucose, glutamate, lactate, and mannose) were significantly decreased after surgery. Interestingly, BCAAs, glucose, and mannose were positively correlated with total cholesterol, LDL cholesterol, triglyceride, which are clinical indicators related to lipid metabolism. In correlation analysis of metabolome and gut microbiome, BCAA metabolites were positively correlated with *Roseburia faecis*. Glycine and dimethyl sulfone were related to *Streptococcus infantis* and *Rothia dentocariosa*. In addition, we performed a quantitative analysis of serum bile acids (BAs) using LC/ triple quadrupole MS (LC/TQ-MS) to measure the level of circulating bile acids reabsorbed in the intestine. After surgery, the total level of BAs increased compared to before surgery. Particularly, GDCA, TDCA, LCA, GLCA, and TLCA, which are secondary BAs, significantly increased after surgery, while primary BAs had little change. This study demonstrates that NMR/MS-based metabolic profiling analysis and it’s integration with microbiome data provides insight into the metabolic changes after bariatric surgery.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) TUE 10:28

Chair: Jongcheol Seo (POSTECH)

Combined Exposure Assessment of Quaternary Ammonium Compounds (QACs) in Various Consumer Chemical Products (CCPs)

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Various biocidal chemicals included in the consumer chemical products (CCPs) have sacrificed many lives and impacted greatly on human health. To effectively regulate the chemicals in the CCPs, the Ministry of Environment have begun to strengthen the regulations on the usage of biocides in the CCPs. One of the most widely used biocidal chemicals in CCPs are quaternary ammonium compounds (QACs). QACs are a group of chemicals having a structure of NR4+, positively charged nitrogen atom with four alkyl chains (R) covalently connected to it. In this research, an analytical method using liquid chromatography tandem mass spectrometry (LC-MS/MS) were applied to identify and quantify 2 different QACs, benzylalkyldimethylethylammonium chloride (BAC), alkyltrimethylammonium bromide (ATMAB). To carry out the exposure assessment, the guidelines suggested by the US Environmental Protection Agency (US EPA) and Korea Ministry of Environment were followed to specify the exposure routes and scenarios. In this research, two different exposure routes, ingestion and dermal contact, were investigated to estimate how much QACs a person is exposed to while using CCPs. QACs in 4 different CCPs, fabric softener, mouthwash, eyedrop and hand sanitizer, were identified and quantified using LC-MS/MS. Furthermore, exposed amount of QACs through various routes were investigated, so that the overall assessment of body exposure to the QACs in the CCP could be estimated.AcknowledgementThis research was supported by a grant (2018002490001) through the Technology Program for Establishing Biocide Safety Management, funded by the Korea Environmental Industry & Technology Institute.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) TUE 10:32

Chair: Jongcheol Seo (POSTECH)

Structural and electrochemical studies of $LiFeBO_3$ as a cathode material for lithium-ion battery

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Lithium iron borate, $LiFeBO_3$, is a particularly desirable cathode material for lithium-ion batteries because of its appealing chemical components, which are inexpensive and non-toxic and its high theoretical capacity of 220 mAh g^{-1}. However, it has low electrical conductivity due to its structural characteristics. Fluorine substitution at the oxygen sites of $LiFeBO_3$ to increase its conductivity and improve electrochemical properties has been studied with phase transition from monoclinic to vonsenite, in previous study. But after the first charge/discharge cycle, it indicate a dramatic decrease of capacity. So, we are studying to improve the stability of its structure by coating at the surface of $LiFeBO_{3-x}F_{2x}$ with maintaining high discharge capacity. The surface coated $LiFeBO_{3-x}F_{2x}$ have been synthesized by solid-state method and characterized by X-ray diffractometry (XRD), TEM images and ^{7}Li MAS NMR spectroscopy. The electrochemical properties of surface coated $LiFeBO_{3-x}F_{2x}$ have been measured by using Galvano static charge/discharge test with the potential range of 1.0 - 4.5 V.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) TUE 10:36

Chair: Jongcheol Seo (POSTECH)

Characteristics and Electrochemical Performance of Silicon/Carbon nanofibers/Graphene Composite films as Anode Material for Binder-Free Lithium ion Secondary Batteries

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

We report the interfacial study of a Silicon/Carbon nanofiber/Graphene Composite material as a potentially high performance anode for rechargeable lithium ion batteries. Carbon Nanofibers (CNFs) were grown using an iron-copper catalysts by the Chemical Vapor Deposition method. Silicon nanoparticles (SiNPs)/Carbon nanofibers (CNFs)/reduced Graphene oxide (rGO) composite films were prepared by simple physical filtration and an environmentally friendly thermal reduction treatment. The films were used as a high performance anode material for self-supporting, binder-free lithium ion batteries. The Silicon nanoparticles were uniformly coated with thermally reduced Graphene oxide (rGO), carbon nanofibers are wound round the surface of the graphene-coated silicon nanoparticles. Reducing graphene oxide has the effect of improving electron conductivity and accommodating volume change during repeated charge/discharge processes. Carbon nanofibers can help maintain structural stability and prevent detachment of silicon nanoparticles from the electrodes. When the produced Si:CNFs/rGO=1:1 composite films was used as an anode of a lithium ion batteries, the initial specific capacity was measured to be 1,894.54 mAh/g at a current density of 0.1 $A\cdot g^{-1}$. After 100 cycles, the reversible specific capacity can be remained at 964.68 mAh/g, the coulombic efficiency can be reached to 93.8% at the same current density. In addition, the SiNPs/CNFs/rGO composite films electrode exhibited a better high specific capacity and cycle stability than an SiNPs/rGO composite films electrode (the reversible specific capacity is 277.28 mAh/g after 100 cycles), the Si:CNFs/rGO=3:2 electrodes (the reversible specific capacity is 545.9 mAh/g after 100 cycles) and the Si:CNFs/rGO=2:3 electrode (the reversible specific capacity is 462.9 mAh/g after 100 cycles). The SiNPs/CNFs/rGO composite films can effectively accommodate and buffer changes of silicon volume, form a stable Solid Electrolyte Interface (SEI), improve the conductivity of the electrode

and provide a fast and efficient channel for electron conduction and ion transport. This technology shows a great promise for the application of anode materials in the field of lithium ion batteries.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) TUE 10:40

Chair: Jongcheol Seo (POSTECH)

Serum exosomes analysis differentiating patients of alcoholic and nonalcoholic fatty liver diseases

Huu-Quang Nguyen, Jaebeom Lee, Jeongkwon Kim*

Department of Chemistry, Chungnam National University, Korea

Exosomes contain many biological materials originated from the releasing cells, including proteins, lipids and RNAs, and are known to be involved in the communication and transferring of components between cells.

In this study, exosomes were enriched from blood serum of patients diagnosed with various states of liver diseases, using multiple centrifugation cycles at 40,000 x g. The enriched exosome samples were analyzed using liquid chromatography tandem mass spectrometry (LC-MS/MS) with Orbitrap mass analyzer. The proteomics data from Orbitrap LC-MS/MS measurements were quantified using MaxQuant software with label-free quantification workflow, followed by univariate and multivariate statistical analysis. By analyzing 24 samples of four different liver disease types, significant differences in protein expression between the diseases, including previously reported markers of liver diseases. Principal component analysis using significantly altered proteins identified from MaxQuant analysis of the LC-MS/MS data provided a confident differentiation between alcoholic and non-alcoholic fatty liver disease groups.

These results provide insight into the use of exosome analysis using mass spectrometry-based proteomics as a tool to assist in diagnosis and prognosis in clinical settings. The new findings open up new possibilities of using mass spectrometry for point-of-care clinical applications as well as for disease discovery and prevention purposes.

Oral Presentation : **ANAL2.O-12**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:44
Chair: Jongcheol Seo (POSTECH)

Homologous recombination repair and cholesterol-mediated drug efflux induce dose-dependent chemoresistance in nutrient-deprived neuroblastoma

Sooyeon Chae, Chae Eun Heo, Min Ji Kim, Chae Ri Park, MyungKook Son, Dongjoon Im, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is a solid pediatric tumor with heterogeneous clinical behaviors. Chemotherapy is widely used to treat neu-roblastoma; however, dose-dependent responses and chemoresistance mechanisms of neuroblastoma cells to anticancer drugs remain challenges in various conditions. Here, we investigated the dose-dependent effects of topotecan on human neuroblastoma cells (SK-N-SH, SH-SY5Y, and SK-N-BE) under various nutrient supply conditions. Serum-starved human neuroblastoma cells showed reduced toxicity, and their survival rate increased upon treatment with a high concentration (1 μM) of topotecan. Quantitative proteomics identified approximately 10,000 proteins in SK-N-SH cells. Network analysis revealed that topotecan up-regulated DNA repair and cholesterol-mediated topotecan efflux, resulting in topotecan re-sistance. Results of cell cycle and quantitative analyses of membrane cholesterol supported the validity of these resistance factors and their applicability to all neuroblastoma cells investigated in this study. Our results provide a model for high dose-dependent chemoresistance in neuroblastoma cells that could enable a patient-dependent chemotherapy screening strategy.

Oral Presentation : **ANAL2.O-13**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:48
Chair: Jongcheol Seo (POSTECH)

An integrated approach for probing quaternary structure change of protein induced by ligand using SAXS and cross-linking/MS

Chae Eun Heo, Chae Ri Park, MyungKook Son, Dongjoon Im, Sooyeon Chae, Minji Kim[1], Hugh I. Kim[*]

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

Characterization of the protein-protein interactions is crucial for the study of a wide variety of biological systems. Numerous research has been reported that various methods are developed to support the identification, characterization, and analysis of protein complexes. Since the protein-protein interactions are easily influenced by post-translational modification (PTM), metal ions, and ion concentration, the development of methods to probe protein-protein interaction induced by environmental factors is needed. Here, we have investigated the ATP effect on the quaternary structure of insulin using multiple biophysical analyses. Firstly, we have conducted the solution small-angle X-ray scattering (SAXS) experiments to understand insulin overall size information, protein association state from their scattering profiles. Then, to identify, characterize, and quantify intermolecular protein-protein interactions in the presence and absence of ATP, we performed crosslinking-mass spectrometry (XL-MS) using two crosslinkers. Finally, we executed molecular docking simulation using our obtained information from the XL-MS regarding residue-residue interaction, and simulated structures were compared to the experimental SAXS profiles to suggest possible protein structures. The experimental methodology using diverse analytical techniques would be highly helpful in understanding the protein-protein interactions.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) TUE 10:52

Chair: Jongcheol Seo (POSTECH)

Proteomic analysis of environmental stress in correlation with physiological changes in *Haliotis discus hannai*

Miseon Jeong, Junghoon Kang, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Korea

With its high market worth and nutrient value for humans, *Haliotis discus hannai*, also known as the Pacific abalone, is a valuable commercial fishery resource in eastern Asia. Various environmental factors, such as temperature, salinity, oxygen, and CO_2 influence its growth and development. Among them, temperature and salinity are the primary physical factors that are affecting the distribution and physiological metabolism of shellfish. These environmentally stressed shellfishes are highly susceptible to pathogens which increase the mortality rate in aquaculture systems. This study aims to determine the physiological changes in *H. discus hannai* by detecting the protein expression of *H. discus hannai* which is influenced by changes in water temperature and salinity. Proteins were extracted with RIPA buffer from homogenized hepatopancreas tissue of *H. discus hannai*. Each supernatant fluid was pooled into experimental and control groups according to the period of exposure to environmental stress. Pooled samples from *H. discus hannai* were trypsin digested and desalted. Subsequently, the proteins in each group were analyzed with nLC-MS/MS and by protein database searches, and then the effect of environmental stress was also determined with differentially expressed protein (DEP) and gene ontology (GO) enrichment analysis.

Oral Presentation : **ANAL2.O-15**
Oral Presentation of Young Analytical Chemists II
Room 301 (Live Streaming) TUE 10:56
Chair: Jongcheol Seo (POSTECH)

Limit of Detection for HPLC-Photodiode Array Detection is Comparable to the Refractive Index Detection for Monosaccharide Analysis.

Iqbal Jalaludin, Jeongkwon Kim*

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High-performance liquid chromatography (HPLC) is most commonly equipped with an ultraviolet (UV) absorbance detectors due to its easy-to-use and good stability qualities. One of the greatest limitations, however, is their failure to produce proper sensitivity for analytes missing a suitable UV chromophore. Refractive Index (RI) detection is indeed an alternate solution to satisfy the former's drawback, while knowing its limitation of using only the isocratic system for HPLC application. UV-absorbance detectors are often overlooked in sugar-related research due to the compounds' low to non-existent UV absorption. However, there is a crucial need to use the gradient method for sugar analysis, since each compound has a unique elution time. In this analysis, we compared the two detection methods for small sugars, i.e. fructose, glucose, sucrose and maltose, to determine the detection limit (LOD). Using the shortest wavelength (190 nm) of our photodiode array detector, the small sugars can be detected. We took this advantage to compare the LOD of the two detection methods, and our preliminary results suggest that the two are comparable for the monosaccharide analysis. This finding shows that UV-absorbance detection can be extended to monosaccharide quantification for quality assurance purposes.

Oral Presentation : **LIFE.O-1**
Oral Presentations by Young Life Chemists
Room 305 (Live Streaming) TUE 09:00
Chair: Hyunsoo Lee (Sogang University)

Detection and screening of biologically active small molecules using a genetically encoded cell-based biosensors

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The ability to screen biologically active small molecules with high sensitivity and specificity is a requirement for biosensing applications. Especially, it is important to screen biological events in their native context for pharmacological and toxicological research. Although in vitro biosensors have been developed and widely used, they often require highly purified probes and targets for screening, thus providing limited information on targets' biological activities in their native environment. To address this issue, we developed a cell-based sensing system that could detect small molecules such as drugs and hormones. We designed a cell-based sensing system using reporter unit based on fluorescence translocation by signal peptide reconstitution. Herein, the signal peptides are activated by conditional protein splicing or conditional protein cleavage without the need for refolding into a functional tertiary structure, thus eliminating false positives and negatives due to mere binding or misfolding. The developed biosensor demonstrated excellent sensitivity and capability to screen the agonist and antagonist of biological target. The developed cell-based sensing system could contribute to improve the screening system aiming to identify the natural mimetics of target and potential drug candidates.

Oral Presentation : **LIFE.O-2**
Oral Presentations by Young Life Chemists
Room 305 (Live Streaming) TUE 09:10
Chair: Hyunsoo Lee (Sogang University)

Structural and biochemical studies of ClpL, an active tetradecameric AAA+ family chaperone

Gyuhee Kim, Sangho Lee*

Department of Biological Sciences, Sungkyunkwan University, Korea

AAA+ (ATPases associated with diverse cellular activities) chaperones are involved in a plethora of cellular activities to ensure protein homeostasis. AAA+ chaperones are major component of Heat shock proteins (HSPs). The functional oligomeric state of AAA+ chaperones is mostly modulated by their hexameric/dodecameric quaternary structures. Here we report the structural and biochemical characterizations of a tetradecameric AAA+ chaperone, ClpL from Streptococcus pneumoniae. We confirmed that ClpL exists as a tetradecamer in solution in the presence of ATP. The cryo-EM structure of ClpL reveals a striking tetradecameric arrangement. Solution structures of ClpL derived from small-angle X-ray scattering data suggest that the tetradecameric ClpL could assume a spiral conformation found in active hexameric/dodecameric AAA+ chaperone structures. Vertical positioning of the middle domain accounts for the head-to head arrangement of two heptameric rings. Biochemical activity assays with site-directed mutagenesis confirmed the critical roles of residues both in the integrity of the tetradecameric arrangement and activities of ClpL. Non-conserved Q321 and R670 are crucial in the heptameric ring assembly of ClpL. These results establish that ClpL is a functionally active tetradecamer, clearly distinct from hexameric/dodecameric AAA+ chaperones.

Oral Presentation : **LIFE.O-3**
Oral Presentations by Young Life Chemists
Room 305 (Live Streaming) TUE 09:20
Chair: Hyunsoo Lee (Sogang University)

Bioinformatic expansion and characterization of Omega-Ester-containing Peptides (OEPs)

Hyunbin Lee, Seokhee Kim[1,*]

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

With the advances in the DNA sequencing techniques and bioinformatic analysis tools, genome mining of natural products has unveiled the wealth and the diversity of their biosynthetic gene clusters in all domains of life. This approach has been successfully applied to the discovery of ribosomally synthesized and post-translationally modified peptides (RiPPs), an intriguing class of natural products. The simple biosynthetic logic of RiPPs demonstrates high potency in bioengineering to generate chemically and topologically diverse molecules with their biosynthetic enzymes. However, enzymatic crosslinkings of two side chains via ester and/or amide bonds have been found only in microviridin, a family of RiPPs, with a single strongly conserved consensus sequence. Here, we discovered ~1,500 new putative microviridin-type RiPPs that can be classified into 12 groups by their core sequence pattern. Connectivities of the six multi-repeat-containing groups were identified by combining tandem mass spectrometry and hydrolysis/methanolysis of esters. Furthermore, we revealed that the ATP-grasp enzymes for these 6 groups are highly specific to the cognate core sequence pattern. Based on our results, we propose the name “Omega-Ester-containing Peptides” (OEPs) to encompass all microviridin-like RiPPs.

Oral Presentation : **LIFE.O-4**
Oral Presentations by Young Life Chemists
Room 305 (Live Streaming) TUE 09:30
Chair: Hyunsoo Lee (Sogang University)

Nanoparticle-Based DNA-Encoded Libraries as a Novel High-Throughput Screening Method for Rapid Discovery of Potent Protein Binding Ligands

Kang ju Lee, Hyun-Suk Lim[*]

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

DNA-encoded libraries (DELs) have been received great interest over the last decade as a valuable high-throughput screening tool, which innovatively accelerate the process of discovering potent protein-binders. In brief, a single DEL member consists of a synthetic compound, a DNA strand to genetically encode the structural information, and a linker to conjugate each component. Tremendous number of different DNA-encoded molecules can be simultaneously screened against target proteins in a single tube. Several successful stories of DELs have been reported in both of the industry and academia including the reports of several drug candidates in clinical trials. In spite of their utility, the reactions for DEL construction should be conducted in aqueous solution, since DNAs are poorly soluble in most of organic solvents. Thereby, the available molecular scaffolds are highly limited in current DEL synthesis. In addition, discovering genuine hit compounds from next generation sequencing often requires complicated and tedious post-sequencing analysis.To overcome such limitations, we developed nanoparticle-based DELs. Owing to solid-phase properties of nanoparticles, most of organic solvents are available for DEL synthesis, which enables to utilize diverse scaffolds. Purification steps are much easier compared to current DELs by using a centrifuge or a magnet. Moreover, multiply displayed encoding DNAs provide more reliable sequencing results. To this end, we synthesized nanoparticle libraries and screened them against target proteins, which provided potent binders with nanomolar affinities. We expect that this on-nanoparticle screening strategy will act as a generally applicable tool for rapid discovery of potent protein binding molecules.

Oral Presentation : **LIFE.O-5**
Oral Presentations by Young Life Chemists
Room 305 (Live Streaming) TUE 09:40
Chair: Hyunsoo Lee (Sogang University)

Enhancing effects of negative-charged liposomes on fibronectin functions in acceleration of wound healing

Huong Thanh Nguyen, Kwanwoo Shin[1,*], Agustina Setiawati[2], Kiyong Lee[3]

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[2]*Department of Life Science, Sogang University, Korea*
[3]*Disease Biophysics Group, John A. Paulson School of Engineering and Applied Sciences, United States*

The unfolded states of fibronectin (FN) eventually induce the formation of the extracellular matrix, which is necessary to generate new tissues. Hence, for the utilization of FN in tissue scaffolding, the demand for a biocompatible material that is capable of stretching compact FN prior to cell delivery is increasing. In this study, we demonstrate that negatively charged small unilamellar vesicles (SUVs) is a qualified candidate for FN delivery due to the enhancement of FN functions in tissue regeneration. Our SUVs were proven to alter the conformation of surface-bound FN greatly. After being delivered to culture cells, the complex of FN-SUV remarkably elevated the attachment, differentiation and migration of fibroblasts. The potential utilization of this complex in drug delivery is also described with a significant healing rate in rats with ulcerative colitis (UC). Altogether, the results suggest that appropriately manufactured FN-SUV could be a novel material not only for wound healing but also for other therapeutic applications.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) TUE 09:50

Chair: Hyunsoo Lee (Sogang University)

Solubilizing and Loading of 1,3-Dicarbonyl Contained Drugs Driven by A Coordinate Interaction

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Interdisciplinary Biosciences and Bioengineering, Pohang University of Science and Technology, Korea

[1]Department of Chemistry, Pohang University of Science and Technology, Korea

To date, numerous polymeric carriers have been developed for effective drug delivery. Generally, those carriers have employed the strategy of self-assembly to load the hydrophobic drug. However, hydrophobic interaction for drug loading is insufficient for high drug loading, colloidal stability, and stimuli-responsive drug release. Therefore, we present a facile strategy to enable solubilizing and loading of drugs utilizing coordinate interaction between drug and phenylboronic acid (PBA). We confirmed reversible interaction between 1,3-dicarbonyl of curcumin (CUR), which is one of a natural drug, and PBA depending on pH. Then, hydrophilic polymer conjugated with PBA (pPBA) was synthesized to solubilize and load CUR via the coordinate interaction. The formation of nano-construct enabled high drug loading (up to 79.2%), uniform size, and colloidal stability, forming a hydrophobic core and hydrophilic shell. Moreover, pH-responsive drug release was achieved, which could enhance anti-cancer effect. As a further study, we confirmed that the strategy utilizing coordinate interaction could be applied to other drugs with 1,3-dicarbonyl (e.g., doxorubicin). Taken together, successful incorporation of the coordinate interaction into drug loading suggests a lot of potential for the platform strategy to enable high drug loading for facile and effective anticancer therapy.

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

Oral Presentations for Young Scholars in Organic Division

Room 306 (Live Streaming) TUE 09:00

Chair: Hong Geun Lee (Seoul National University)

Atroposelective Total Syntheses of *M*- and *P*-Naphthylisoquinoline Alkaloids Using an Internal Central Chirality

Young-In Jo, Cheol-Hong Cheon[*]

Department of Chemistry, Korea University, Korea

Since naphthylisoquinoline alkaloids exhibit interesting biological activities and structural diversities, they have received considerable attention from the synthetic and medicinal communities. However, these natural products possess both central and axial chiralities, and thus they have been considered synthetically challenging targets. Although numerous methodologies to control central chirality have been reported, approaches to control the axial chirality have been far less developed. In addition, since most of the previous syntheses have been designed for the synthesis of specific target molecule, it was difficult to synthesize naphthylisoquinoline alkaloids with structural diversity Furthermore, previous approaches have been limited to the synthesis of one atropodistereomer, and there are no reports of the synthesis of two atropisomers on the same substrate.Recently, our group reported the asymmetric total syntheses of ancistrocladinium A, one of the N,C-coupled naphthylisoquinolines, and its atropdiastereomer via diastereoselective construction of axial chirality using the central chirality at the C-3 position of the isoquinoline ring.1,2 As a part of our research program toward the atropselective synthesis of naphthylisoquinoline alkaloids, we investigated the atropselective synthesis of C,C-coupled naphthylisoquinoline alkaloids using the internal central chirality existing in the isoquinoline ring.3 In this presentation, we will describe the asymmetric total syntheses of several naphthylisoquinoline alkaloids via atroposelective Suzuki-Miyaura coupling reaction. Reference1.Kim, K.-H.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 28832.Kim, K.-H.; Cheon, C.-H. Org. Chem. Front. 2017, 4, 13413.Jo, Y.-I.; Lee, C.-Y.; Cheon, C.-H. Org. Lett. 2020, 22, 4653

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

Oral Presentations for Young Scholars in Organic Division

Room 306 (Live Streaming) TUE 09:12

Chair: Hong Geun Lee (Seoul National University)

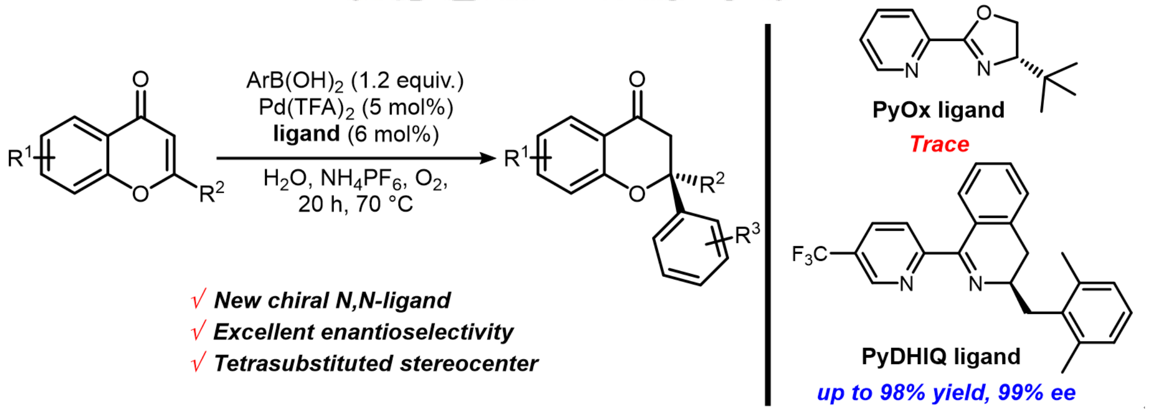
Catalytic Enantioselective Synthesis of Tetrasubstituted Chromanones via Palladium-Catalyzed Asymmetric Conjugate Arylation Using Chiral Pyridine-Dihydroisoquinoline Ligands

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*

Highly enantioselective conjugate addition reactions of arylboronic acids to 2-substituted chromones catalyzed by palladium complexes with new chiral Pyridine-Dihydroisoquinoline (PyDHIQ) ligands have been developed. These reactions provide highly enantioselective access to chromanones containing tetrasubstituted stereocenters. Various arylboronic acids and 2-substituted chromones can be used in the catalytic reaction to afford the chiral tetrasubstituted chromanones in good yields and excellent enantioselectivities (25 examples, up to 98% yields, up to 99% ee).



Oral Presentation : **ORGN.O-3**
Oral Presentations for Young Scholars in Organic Division
Room 306 (Live Streaming) TUE 09:24
Chair: Hong Geun Lee (Seoul National University)

Molecular Mechanism of Viscosity Sensitivity in Motion-Based BODIPY Rotors

Xiao Liu, Young-Tae Chang[1,*]

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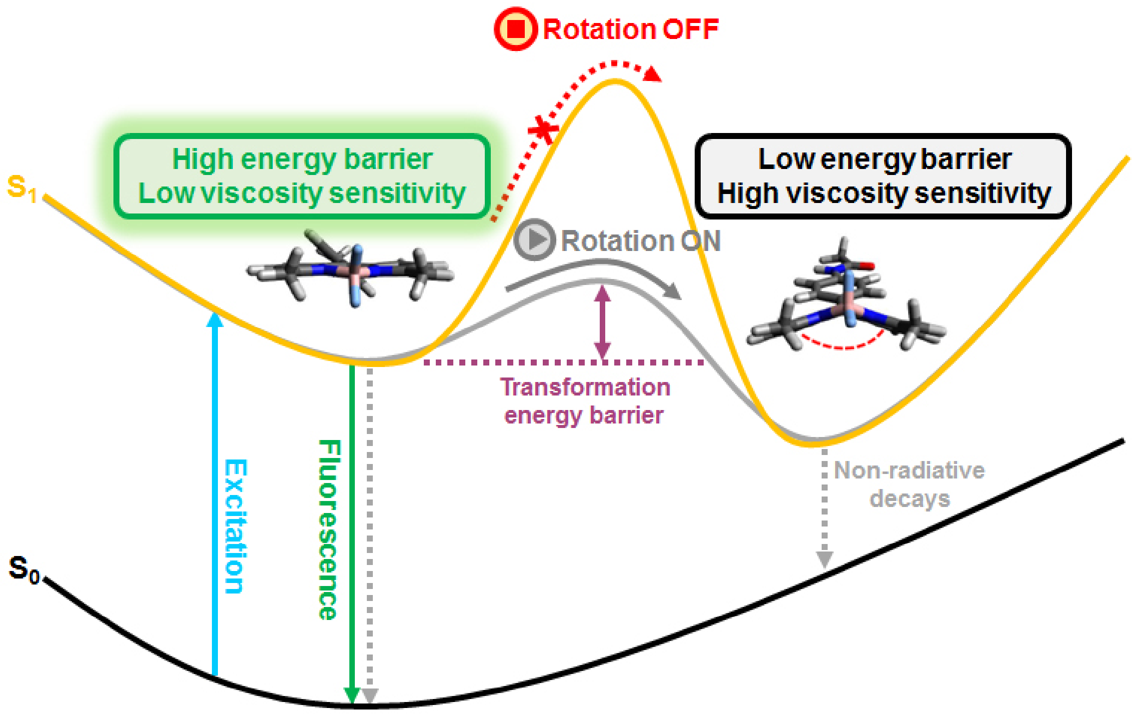
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Viscosity in the intracellular microenvironment shows a significant difference in various organelles and is closely related to cellular processes. To better understand bioprocess in live cells, it is necessary to dynamically monitor or map the intracellular viscosity in their native state. For this purpose, various fluorescent molecular rotors have been widely exploited to study intracellular microenvironment, where BODIPY rotors are one of the cases. However, the relationship between the molecular structures of the various compounds and their effect on viscosity sensitivity remains mostly unaddressed. Understanding such a mechanistic relationship is, however, critical for the effective design of improved viscosity sensors.Herein, we systematically synthesized and investigated two sets of BODIPY-based molecular rotors to study the relationship between intramolecular motions and viscosity sensitivity. Through experimental and computational studies, two conformations (i.e., the planar and butterfly conformations) are found to commonly exist in BODIPY rotors. We demonstrate that the transformation energy barrier from the planar conformation to the butterfly conformation is strongly affected by the molecular structures of BODIPY rotors, and is inversely correlated with the viscosity sensitivity. These findings enable rational structure modifications of BODIPY molecular rotors for highly effective protein detection and recognition.


Rotation OFF
S1
High energy barrier
Low viscosity sensitivity
Rotation ON
Low energy barrier
High viscosity sensitivity
Transformation energy barrier
Excitation
Fluorescence
Non-radiative decays
S0

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

Oral Presentations for Young Scholars in Organic Division

Room 306 (Live Streaming) TUE 09:36

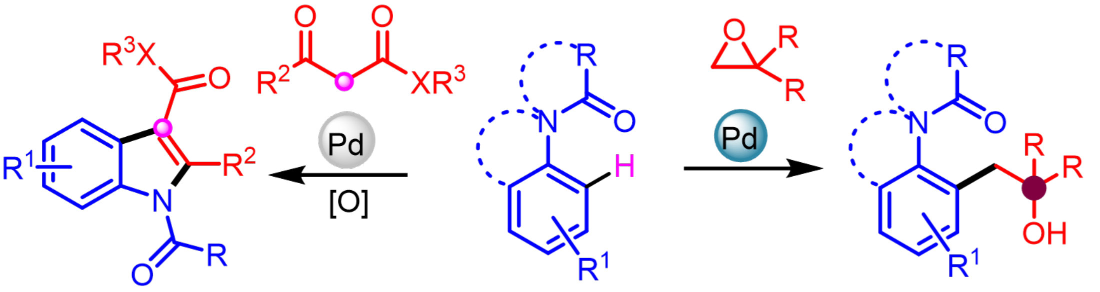
Chair: Hong Geun Lee (Seoul National University)

Palladium-Catalyzed C-H Functionalization of Acetanilides

Raju Sitaram Thombal, Yong Rok Lee*

Chemical Engineering, Yeungnam University, Korea

In the recent decade, palladium-catalyzed C–H functionalization reactions have become powerful transformations for the construction of C–C bonds. Palladium-catalyzed direct activation of the aromatic CSp2–H bonds is one of the frontier areas in organic chemistry, and the progress of research in this field is very rapid. Compared with other transition metals, palladium has the advantages of high catalytic activity and strong selectivity. In the context of directed C-H functionalization, the acetanilide has been used as a successful substrate with the easily removable acetyl as a directing group (DG). Recently, we have disclosed the two elegant methodologies using acetanilide and □-keto esters or epoxides as coupling partners under palladium catalysis (Scheme 1). The focus of these works is directed towards the synthesis of biologically interesting heterocycles. These novel Pd(II)-catalyzed C–H activation protocols include (1) C(sp3)−H/C(sp2)−H coupling/annulation of anilides and α-dicarbonyl compounds for the synthesis of diverse N-acyl indoles and (2) C–H functionalization of acetylated anilines (acetanilides, 1,1-dimethyl-3-phenylurea, 1- phenylpyrrolidin-2-one, and 1-(indolin-1-yl)ethan-1-one) with epoxides.



Org. Lett. **2020**, *22*, 3397

- Direct oxidative C-H activation
- High regioselectivity
- Pre-activation not required
- Broad substrate scope

Chem. Sci. **2020**, *11*, 7260

- Detailed experimental and computational studies
- Compatible with various DG and chiral epoxides
- 25 examples, up to 81% yield

Scheme 1. Pd(II)-catalyzed C-H functionalization of acetanilides with β-keto esters or epoxides

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

Oral Presentations for Young Scholars in Organic Division

Room 306 (Live Streaming) TUE 09:48

Chair: Hong Geun Lee (Seoul National University)

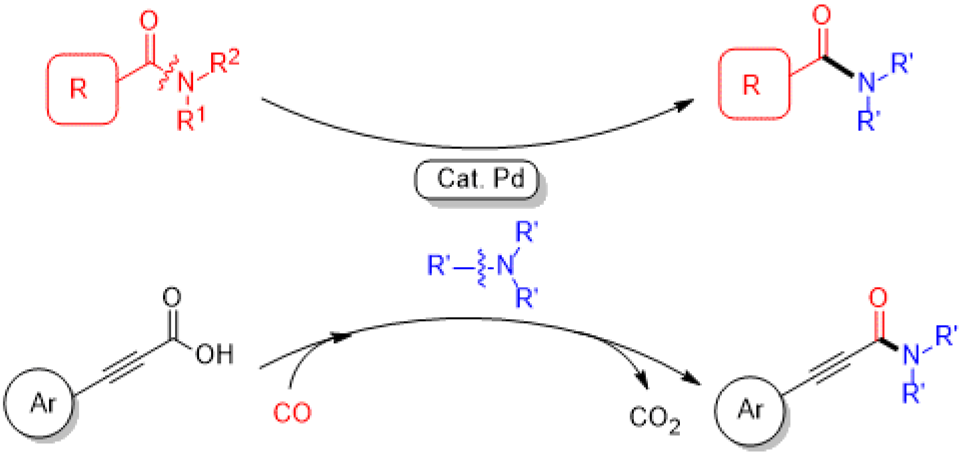
HARNESSING THE C-N BONDS OF TERTIARY AMINES/AMIDES IN AMINOCARBONYLATION AND TRANSAMIDATION REACTIONS

Muhammad Aliyu Idris, Sunwoo Lee[1,*]

Chemistry, Chonnam National University, Korea

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

It is a well-established fact that the C-N bond is amongst the ubiquitous chemical bonds found in organic molecules and biomacromolecule. However, these bonds are not so easy to manipulate owing to the high C-N bond dissociation energy. Thus, it is of paramount importance to indulge into discovering various protocols to harness them. Herein, are two different methodologies involving the activation/cleavage of an inert C-N bond in tertiary amines and in twisted amide. The first transformation is a palladium catalyzed decarboxylative aminocarbonylation of alkynoic acids with tertiary amines where oxygen was found to be crucial in the cleavage of the inert C-N bond in the tertiary amines. And, the second protocol is a transamidation involving a double C-N bond cleavage of tertiary amine and a twisted amide. It proceeds via palladium catalysis coupled with DTBP (an oxidant) which we believed to have a crucial impact on the C-N bond cleavage.


O
R
N
R2
R1
R'
Cat. Pd
OH
Ar
CO
CO2

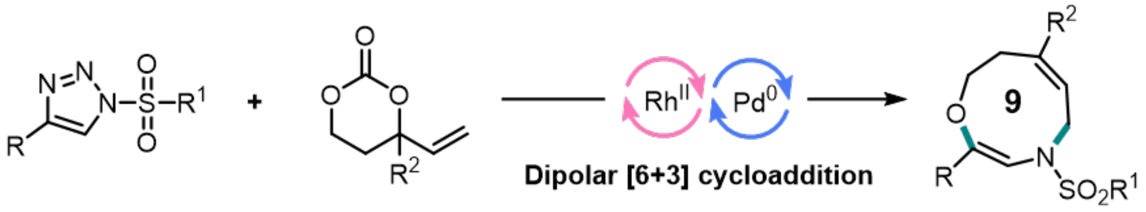
Oral Presentation : **ORGN.O-6**
Oral Presentations for Young Scholars in Organic Division
Room 306 (Live Streaming) TUE 10:00
Chair: Hong Geun Lee (Seoul National University)

Synthesis of 9-Membered 1,4-Oxazonines via Synergistic Rh(II)/Pd(0) Dual Catalysis

Kyu Ree Lee, Subin Ahn, Sang-gi Lee[1,*]

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

Medium-sized heterocycles are ubiquitous in biologically active compounds. However, synthetic strategy for these heterocyclic molecules is still limited.[1] During our ongoing study on the cooperative dual catalysis,[2] we envisioned that 9-membered heterocyclic 1,4-oxazonines could be synthesized through the synergistic Rh(II)/Pd(0) dual catalytic [6+3] dipolar cycloaddition reaction between the catalytically generated reactive intermediates, i.e., 1,3-dipole equivalent α-imino Rh-carbenoid formed from *N*-sulfonyl-1,2,3-tirazoles **1** and 1,5-dipole equivalent zwitterionic alkoxy π-allyl Pd(II)-complex formed from 4-vinyl-1,3-dioxan-2-one **2**.Reference[1] (a) Yet, L. *Chem. Rev.* **2000**, *100*, 2963. (b) Vo, C.-V. T.; Luescher, M. U.; Bode, J. W. *Nat. Chem.* **2014**, *6*, 310.[2] (a) Chen, Z.-S.; Huang, L.-Z.; Jeon, H. J.; Xuan, Z.; Lee, S.-g. *ACS Catal.* **2016**, *6*, 4914. (b) Huang, L.-Z.; Xuan, Z.; Jeon, H. J.; Du, Z.-T.; Kim, J. H.; Lee, S.-g. *ACS Catal.* **2018**, *8*, 7340.



1 **2** **1,4-Oxazonine**

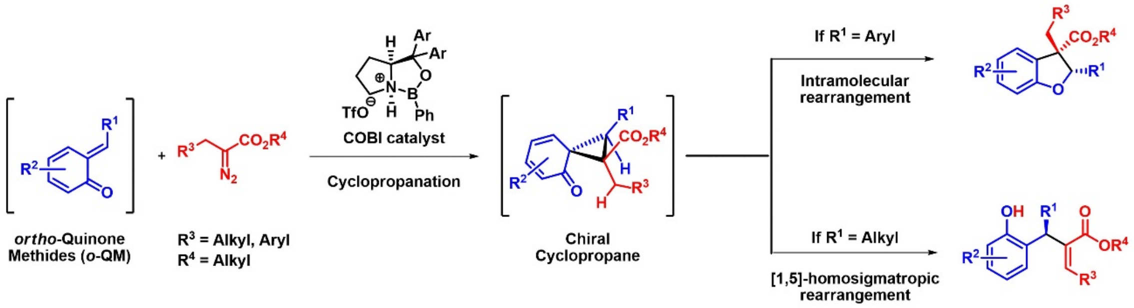
Oral Presentation : **ORGN.O-7**
Oral Presentations for Young Scholars in Organic Division
Room 306 (Live Streaming) TUE 10:12
Chair: Hong Geun Lee (Seoul National University)

Lewis Acid Catalyzed Tandem Reactions Using ortho-Quinone methides.

Seung Tae Kim, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

ortho-Quinone methides (o-QM) has a cyclohexadiene structures with exocyclic alkene and carbonyl group, which positioned by ortho to each other. It has attracted great scientific interests in recent decades because of high reactivity and used as important intermediates in organic synthesis.[1]Chiral oxazaborolidinium ion (COBI) catalyst is the one of the Lewis acid catalysts, used to proceed many reactions having carbonyl or imine compounds. In this research, we developed the enantioselective synthesis of 2,3-dihydrobenzofurans and α-methylene carbonyl compounds, also known as Rauhut-Currier type products, via tandem reactions catalyzed by COBI catalyst. Intermediate chiral cyclopropane was formed by reaction of o-QM with diazo compounds under COBI catalyst, giving 2,3-dihydrobenzofuran possessing quaternary carbon center in the case of R1 = aryl groups[2] and Rauhut-Currier type products through [1,5]-homosigmatropic rearrangement when R1 was alkyl groups.[3]References1. (a) Z. Wang, J. Sun, Synthesis 2015, 47, 3629-3644; (b) C. D.-T. Nielsen, H. Abas, A. C. Spivey, Synthesis 2018, 50, 4008-4018.2.R. P. Pandit, S. T. Kim, D. H. Ryu, Angew. Chem. Int. Ed. 2019, 58, 13427-13432. 3.Manuscript in preparation.



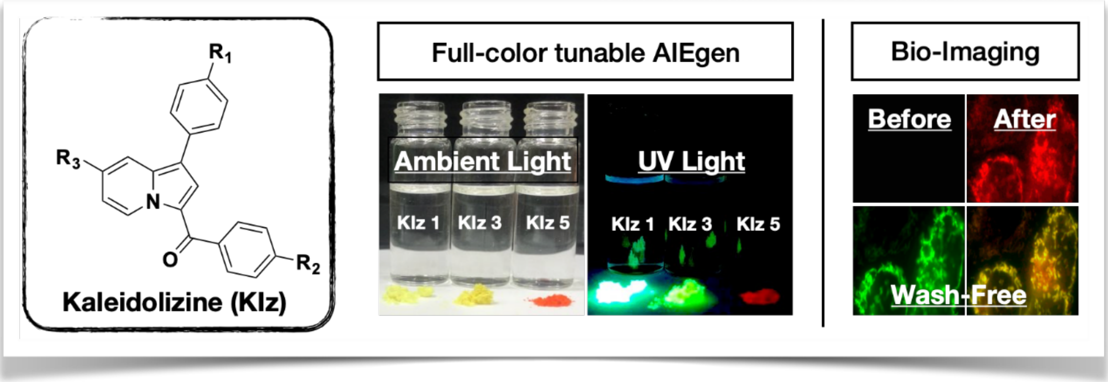
Oral Presentation : **ORGN.O-8**
Oral Presentations for Young Scholars in Organic Division
Room 306 (Live Streaming) TUE 10:24
Chair: Hong Geun Lee (Seoul National University)

Full-color tunable aggregation-induced emission fluorophore based on indolizine

Sang-Kee Choi, Hyungi Kim, Jun-Sik Min[1], Seulbi Lee[1], Eunha Kim[*]

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

Fluorescent fluorophore was used in various field because of its sensitive property. But conventional fluorophores have aggregation-caused quenching(ACQ) phenomena when they aggregate. So they have some problems to apply on practical applications. To overcome the problems, the opposite method should be introduced that weakly luminescent chromogens in solution state are induced to give high fluorescent signal by the aggregate formation. That is called ‘Aggregation-Induced Emission(AIE)’. Only a limited number of organic fluorescent dyes have been reported as representing AIE characteristics. However, several Kaleidolizine derivatives have low fluorescent intensity in solution state but have high fluorescent intensity in their solid state. AIE probes have ultrahigh imaging contrast, good photostability, and increased intensity with low concentration. Between intramolecular charge transfer (ICT) and restriction of intramolecular rotation (RIR) act as the AIE mechanism in the KIz system. Modification of triphenylphosphonium(TPP) on Kaleidolizine allows successful development of fluorogenic probes for real-time bio-imaging of mitochondria in cells.


R1
R3
N
O
R2
Kaleidolizine (Klz)
Full-color tunable AIEgen
Ambient Light
Klz 1
Klz 3
Klz 5
UV Light
Klz 1
Klz 3
Klz 5
Bio-Imaging
Before
After
Wash-Free

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

Oral Presentation for Young Material Chemists

Room 304 (Live Streaming) TUE 09:00

Chair: Soo Min Kim (Sookmyung Women's University)

Near-Infrared Emissive Iridium(III) Complexes with Aggregation-Induced Phosphorescence Enhancement

Hae Un Kim, Kyoungwon Choi, Taehyun Kim, Dohyun Kim, Taiho Park[*]

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

Triplet–triplet annihilation and vibrational deactivation are exhibited mainly in low bandgap phosphorescent emitters. Near-infrared (NIR) emissive iridium(III) complexes showing aggregation-induced phosphorescent enhancement (AIPE) are designed and synthesized by anchoring electron-withdrawing substituents on the N-coordinating quinoline moiety of a (benzo[*b*]thiophen-2-yl)quinoline cyclometalated ligand along with ancillary picolinate. The origin of AIPE and excited-state properties of the complexes are thoroughly investigated with the utilization of density functional theory calculation and single-crystal X-ray diffraction analysis. The complexes are employed for the fabrication of NIR OLEDs by hybrid solution-process, achieving maximum external quantum efficiency (EQE) of 7.29%.

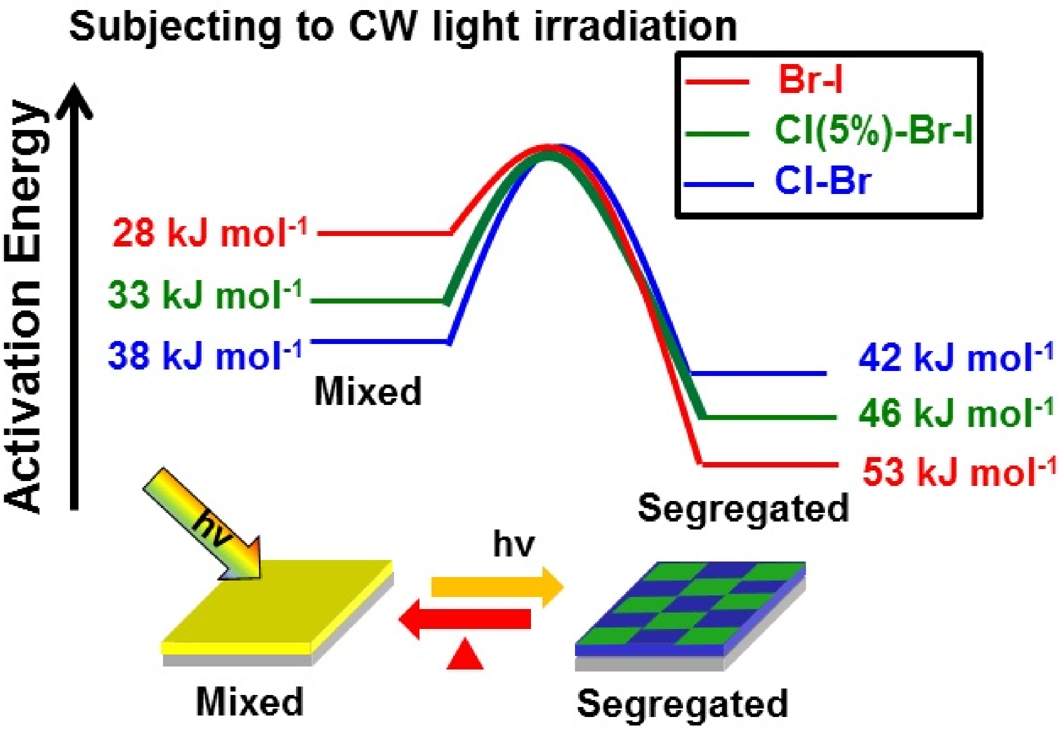
Oral Presentation : **MAT.O-2**
Oral Presentation for Young Material Chemists
Room 304 (Live Streaming) TUE 09:15
Chair: Soo Min Kim (Sookmyung Women's University)

Fate of Photoinduced Halide Ion Segregation and Iodide Expulsion: Thermodynamic and Kinetic Aspects

Junsang Cho

Department of Chemistry, Duksung Women's University, Korea

Suppression of halide ion mobility, governing the device performances and stability, remain a key issue for designing for the stable perovskite solar cells. The halide ion migration facilitated by the lattice-distortion-mediated halide vacancy formation is known as influenced by polarizability (or rigidity) of the halide sublattice and framework. Here, we have probed photo-induced halide ion segregation and dark recovery using MAPb(Cl0.5Br0.5)3 films. The temperature dependence of the rate constants (in Arrhenius plot) allows for determining the activation energy barriers (Ea) for photosegergation (38 kJ/mol) and dark recovery (42 kJ/mol), respectively. A comparison of the segregation activation energy (Ea) and excitation intensity threshold between MAPb(Cl0.5Br0.5)3 and MAPb(Br0.5I0.5)3 films reflects that incorporation of Cl into halide sublattices allows for stabilizing the mixed halide composition as a result of thermodynamic stabilization by forming more rigid [PbX6]4- frameworks with an increased barrier for halide ion migration. The thermodynamic rationale behind intriguing halide ion mobility offers a fundamental insight into the role of Cl and design principle of perovskite solar cells with improved efficiency and long-term stability.**References***1. Cho, J.; Kamat, P.V. Chem. Mater. 2020, 32, 6206–62122. Cho, J.; DuBuse, J. T.; Le, A. N. T.; Kamat, P. V. ACS Materials. Lett. 2020, 2,565-5703.Cho, J.; Kamat, P. V. Thermodynamic Rationales behind Cl-Br Halide Ion Segregation, submitted to Adv. Opt. Mater. 2020*3. *4. Cho, J.; DuBose. J. T.; Matthew. P. S.; Kamat, P. V. Electrochemical Insight of Role of Chloride into Stabilization of Mixed Halide Perovskites, Manuscript in Preparation*


Subjecting to CW light irradiation
Activation Energy
Br-I
Cl(5%)-Br-I
Cl-Br
28 kJ mol-1
33 kJ mol-1
38 kJ mol-1
Mixed
42 kJ mol-1
46 kJ mol-1
53 kJ mol-1
Segregated
hv
hv
Mixed
Segregated

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

Oral Presentation for Young Material Chemists

Room 304 (Live Streaming) TUE 09:30

Chair: Soo Min Kim (Sookmyung Women's University)

Facile and high-throughput screening of direct-acting antiviral drug with graphene oxide-based fluorescent biosensor

Se-Jin Park, Dal-Hee Min*

Department of Chemistry, Seoul National University, Korea

Dengue virus (DV) is a mosquito-borne, human-pathogenic RNA virus that belongs to the family of Flaviviridae. Severe progression of DV infection may induce life-threatening symptoms such as hemorrhagic fever and dengue shock syndrome, with a rapid decline in platelet counts and bleeding. The recent DV outbreak has shown a tendency to expand worldwide, mainly due to the rapid globalization. Meanwhile, the concept of a direct-acting antiviral agent has drawn much attention for its potent, promising therapeutic effect. Associated with this, RNA-dependent RNA polymerase (RdRp), an RNA virus-specific enzyme highly conserved among various viral families, has been known as the broad-range target suitable for the discovery of such. To date, however, only limited methods exist to discover RdRp inhibitors. Conventional RdRp-associated assays include gel electrophoresis or radioactive labels, which are not compatible with the high-throughput screening due to laborious, time-consuming procedures and high cost. Here, we introduce the development of a nanobiosensor incorporating RNA and graphene oxide (RNA-Nano-Graphene Oxide system, abbreviated as RANGO) to enable the quantitative analysis of the RNA virus-specific enzyme activity based on fluorescence, and its application to a high-throughput chemical screening to identify a novel direct-acting antiviral agent against RNA virus from the FDA-approved small molecule library.

Oral Presentation : **MAT.O-4**
Oral Presentation for Young Material Chemists
Room 304 (Live Streaming) TUE 09:45
Chair: Soo Min Kim (Sookmyung Women's University)

Reduced graphene oxide-based composites toward attenuation of high frequency range electromagnetic wave

Quyen Vu thi, Daewon Sohn*

Department of Chemistry, Hanyang University, Korea

Nowadays, the extensive use of portable and wearable smart electronics brings to the forefront the increasing of electromagnetic interference (EMI) to our living space, causing a demand forward in developing flexible absorbing materials with outstanding absorption efficiency, lightweight density, anticorrosion and easy proceeding. Since the first successful synthesis of graphene in year 2004, graphene has been widely applied in materials science filed including EMI application due to its extraordinary properties such as ultra-specific surface area, high mechanical strength and ultra-low density. However, graphene or its most common derivative named reduced graphene oxide (rGO) owing a high electrical conductivity, exhibit an impedance mismatch, causing the limitation of microwave-absorbing power. Therefore, it is still remaining challenges to improve the EMI absorbing capability of graphene or rGO-based composite in the field of EMI shielding application. In this talk, we are going to provide strategies to maximize absorption performance of reduced graphene oxide by combining with other losing components such as conducting polymers, magnetic compounds and porous materials. The massive enhancement in EMI performance will be clarified with detail mechanism in the talk.

Oral Presentation : **MAT.O-5**
Oral Presentation for Young Material Chemists
Room 304 (Live Streaming) TUE 10:00
Chair: Soo Min Kim (Sookmyung Women's University)

Specific detection of Zika and dengue viruses with graphene oxide-based biosensor

Ji-Seon Lee, Dal-Hee Min*

Department of Chemistry, Seoul National University, Korea

Due to the global warming and climate change, spread of flavivirus which is transmitted by mosquito vectors has threatened the human worldwide. Zika and dengue viruses are closely related flaviviruses which have a similarity in genetic information. It has been reported that co-infection between those viruses cause the severe diseases. Thus, rapid and accurate diagnosis of each virus (ZIKV and DENV S1-S4) is crucial to prevent the risks from repeated virus infections. Here, we report a graphene oxide-based molecular diagnostic strategy for multiplexed detection of relevant flaviviruses, ZIKV and DENVs by targeting viral genome. Specifically, we combined the PNA/GO-based biosensor with loop-mediated isothermal amplification (LAMP). During the amplification of viral RNA, single-stranded loops of the virus amplicon is produced, and fluorescent PNA probes can recognize them through target-probe hybridization. Meanwhile, graphene oxide can selectively distinguish and quench the fluorescence of unbound PNA driven by its preferential interaction with single-stranded nucleic acid over double-stranded one. This strategy facilitates differential diagnosis of similar viruses with distinctive specificity, and shorten the manual step of nucleic acid testing (NAT) by integrating the RNA extraction and amplification process of virus sample.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 408 (Live Streaming) TUE 09:00

Chair: Chang Hyuck Choi (GIST)

Electrochemical Analysis of Single Water Droplets using Outer Sphere Reaction

Heekyung Park, Jun Hui Park*

Department of Chemistry, Chungbuk Natioanl University, Korea

We report the electrochemical detection of single water droplets in organic solvent using a ultramicroelectrode (UME). Our previous study observed water droplet in organic solvent using water oxidation reaction. However, the oxidation of water proceeds about 0.81 % inside the water nano-droplet due to the pH change from the reaction product H^+. Using the outer sphere redox species which have lower oxidation potential, we could achieve the 100 % oxidation of the redox species dissolved in nano-droplet. The water droplets were detected by amperometric i-t curve. The applied potential was determined by measured cyclic voltammetry organic solvent against aqueous solution to background current and redox potential range, respectively. The size of emulsion included redox species by charge integration has been well match with measured DLS data. The current spike shapes were sharp increased rapidly and then exponentially decay, and it analyzed using a bulk electrolysis model. The droplet size was small enough to assume that the mass-transfer of the redox species in nano-droplet was fast enough. Simulated current decay fitting data showed a very small contact area compared to the droplet size.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 408 (Live Streaming) TUE 09:15

Chair: Chang Hyuck Choi (GIST)

Electrochemical detection of redox-free single water droplets in organic solvent

Hyeong kwon Moon, Jun Hui Park*

Department of Chemistry, Chungbuk Natioanl University, Korea

We report the electrochemical detection on water-in-oil emulsion droplet by collision oxidation of AA extracted from continuous phase using a platinum ultramicroelectrode (Pt-UME) without hydrophobic electrolyte. In this experiment, water droplets were prepared by the ultrasonication of organic solvent (e.g., dichloroethane) containing dioctyl sulfosuccinate (AOT) as an emulsifier and aqueous solution containing sodium chloride as a hydrophilic electrolyte. Incubating for few minutes, enough of time to AA be extracted, the spike-shaped current peak resulted from electrochemical reaction of water droplet observed in the chronoamperometry over the oxidative potential of redox species. Single water droplet that collides with the Pt-UME led to amperometric current spike peak due to the instantaneous electrolysis of the redox species. The charge of single collision events was proportional to the droplet size and concentration of redox species. By adjusting the concentration of the AA, the size of single water droplet were estimated. Moreover, the contact area of the droplet can be obtained. We could successfully establish a new pure water droplet detection system in organic solvent.

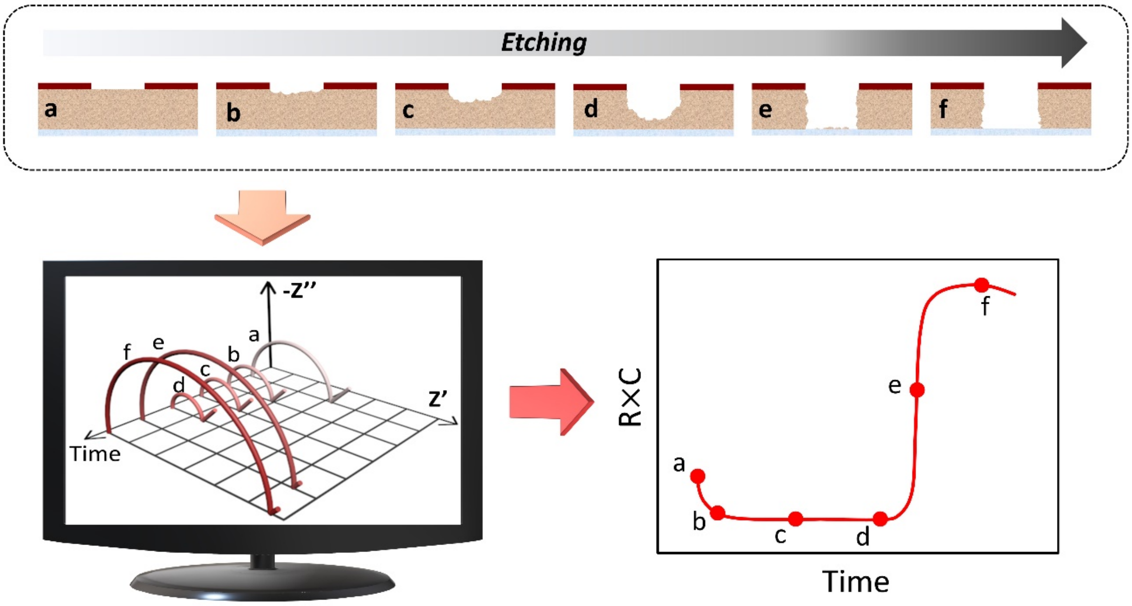
Oral Presentation : **ELEC.O-3**
Oral Presentation of Young Scholars in Electrochemistry
Room 408 (Live Streaming) TUE 09:30
Chair: Chang Hyuck Choi (GIST)

In Situ Real-time Monitoring of Chemical Etching Process of ITO Film via Fourier-transform Electrochemical Impedance Spectroscopy

Seok Hee Han, Taek dong Chung[*]

Department of Chemistry, Seoul National University, Korea

Electrochemical impedance spectroscopy (EIS) has been deemed a powerful technique which gives a full knowledge of the electrode surface including faradaic and non-faradaic aspects. Fourier-transform electrochemical impedance spectroscopy (FT-EIS) allows us a time-resolved investigation of electrochemical systems, whereas conventional EIS is not applicable owing to its long measurement time. Here, we implemented FT-EIS using step-excitation signal for an in situ, real-time analysis during the entire chemical etching process of ITO film electrode under $FeCl_3$-HCl solution, which is frequently used in most cases. We successfully visualized the electrochemical activation of ITO electrode as the etching progressed, as well as the completion of the process by continuously monitoring the fluctuation of equivalent circuit parameters, i.e. charge transfer resistance (R_{ct}), double layer capacitance (C_{dl}), which were simultaneously calculated from the FT-EIS data. We verified a similar tendency in electrochemical aspects from the cyclic voltammograms and impedance data obtained from ferri- and ferrocyanide redox couple. We further applied this technique to procure undamaged interdigitated array (IDA) bearing more delicate patterns by preventing the excessive etching. The technique could also be used to optimize the etching procedure, or to prepare electrodes with desired activity, and even to screen out abnormalities. This work lets us rediscover the potential of FT-EIS enabling in situ real-time electrochemical examinations in other constantly changing, transient systems such as electrodeposition, corrosion and surface modification.



In Situ, Real-time FT-EIS Analyzer

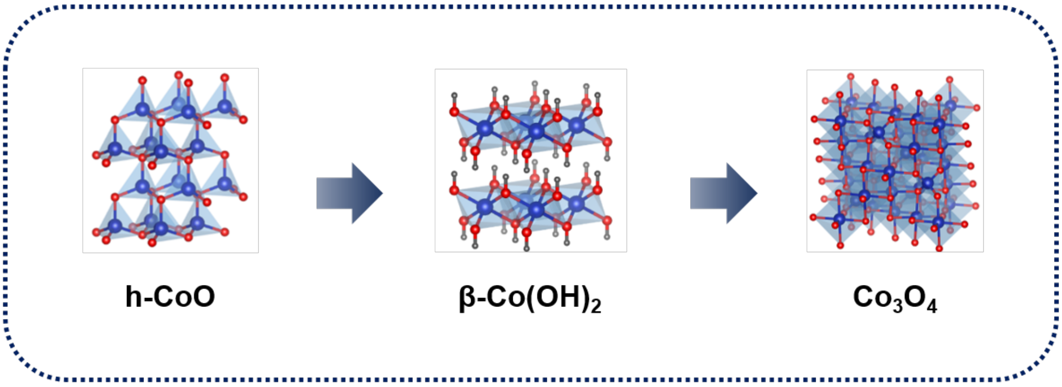
Oral Presentation : **ELEC.O-4**
Oral Presentation of Young Scholars in Electrochemistry
Room 408 (Live Streaming) TUE 09:45
Chair: Chang Hyuck Choi (GIST)

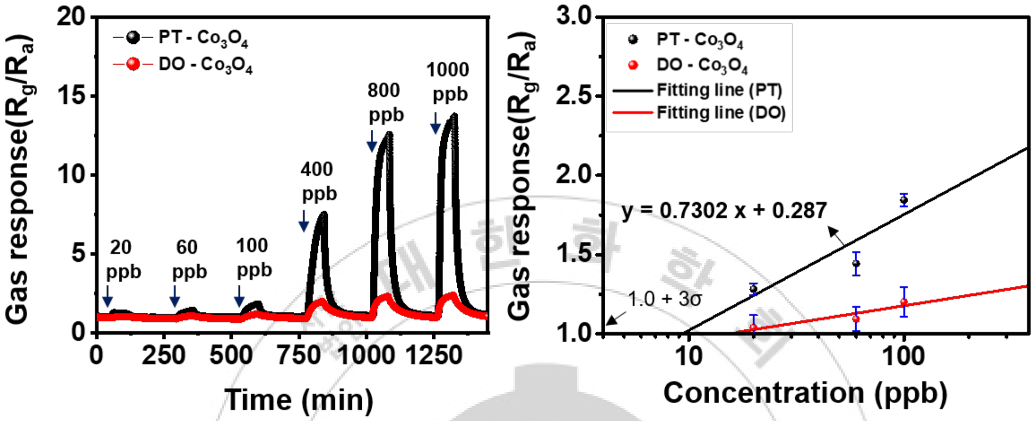
Semiconductor electrochemistry: Application to ultrasensitive acetone gas sensor.

Ahyeon Ma, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

Semiconducting metal oxides are known for years as efficient gas sensing elements, since their electrical conductivity varies greatly with the changes in surrounding gas atmosphere. The development of sensing materials with high sensitivity and selectivity, which influence the practical gas-sensing performance, is critically important for the further evolution of semiconducting metal-oxide gas sensors. Herein, a nanoscale sensing material was prepared in a facile manner via the phase transition of wurtzite CoO to spinel Co3O4, as a new gas sensor preparation platform. The combination of a h-CoO → β-Co(OH)2 phase transition followed by thermal oxidation led to the spontaneously deposition of Co3O4 on the interdigitated electrodes (IDEs). The prepared Co3O4 nanoplates exhibited good contact adhesion with the sensor substrate, which obviated the need for conventional film forming processes, and were shown to be suitable for direct gas sensing. Compared to other Co3O4 sensors, the phase-transitioned Co3O4 nanoplates show very high sensitivity to acetone gas (12.5 for 1 ppm acetone) in the range of 20-1000 ppb at an operating temperature of 200 ℃ and enhanced selectivity. The improved performance of the Co3O4 nanoplates is attributed to typical crystal facets with mainly exposed (111) planes as well as an enlarged surface area during phase transition. Therefore, it was concluded that phase transition methods can be applied to promising sensing substance to develop a variety of related ultrasensitive acetone sensors.


h-CoO
β-Co(OH)$_2$
Co$_3$O$_4$


Gas response(R$_g$/R$_a$)
PT - Co$_3$O$_4$
DO - Co$_3$O$_4$
20 ppb
60 ppb
100 ppb
400 ppb
800 ppb
1000 ppb
0
5
10
15
20
0
250
500
750
1000
1250
Time (min)
Gas response(R$_g$/R$_a$)
PT - Co$_3$O$_4$
DO - Co$_3$O$_4$
Fitting line (PT)
Fitting line (DO)
y = 0.7302 x + 0.287
1.0 + 3σ
1.0
1.5
2.0
2.5
3.0
10
100
Concentration (ppb)

Oral Presentation : **ELEC.O-5**
Oral Presentation of Young Scholars in Electrochemistry
Room 408 (Live Streaming) TUE 10:00
Chair: Chang Hyuck Choi (GIST)

Monitoring the respiration activity of single neural stem cells using scanning electrochemical microscopy (SECM)

Dong Hoon Im, Hyun Seo Ahn[1,*]

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

Cellular respiration is one of the important metabolism of life. How this varies by cell type should be analyzed. In particular, the heterogeneity of cells should be revealed from the perspective of single-cell research, which has made much progress recently. In this work, we are observing the respiration of single stem cell by using scanning electrochemical microscopy (SECM) to approach the cell with nanoelectrodes. We will find out how they differ depending on the differentiation step, what is the heterogeneity between cells, and how they relate to the final differentiation outcome.

Oral Presentation : **ELEC.O-6**
Oral Presentation of Young Scholars in Electrochemistry
Room 408 (Live Streaming) TUE 10:15
Chair: Chang Hyuck Choi (GIST)

Capping-ligand effect of copper nanoparticles for electrochemical reduction of carbon dioxide

Yusik Oh, Hye Ryung Byon*

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., C2+) products. Copper (Cu) is known as the sole catalyst to yield C2+ products by affording the suitable binding energy to the intermediate of *CO (the asterisk denotes the surface adsorption). Although various synthetic methods for the preparation of Cu nanoparticles (NPs) have been developed to increase the surface area and design of the preferred facets for the CO_2 reduction, the highly sensitive Cu surface in air and from contaminants resulted in variable Faradaic efficiencies for C2+ production. In particular, the capping ligands, which coat the Cu surface to stabilize the designed nanostructures, should significantly influence the catalytic efficiency and stability. However, their effects have been little studied. Here, we show the enhanced catalytic activity and stability of Cu NPs for the C2+ yield by eliminating the capping ligands. The pristine Cu NPs with ~8 nm of diameter were prepared by using a capping ligand of tetradecylphosphonate (TDP). After UV-ozone treatment, the TDP ligands were eliminated in part; The phosphorous signal was attenuated, and the Cu surface was oxidized in X-ray photoelectron spectra. In addition, the carbonyl oxygen (O=C) emerged from the damaged TDP. In contrast, the carbon substrate and the surface roughness of the Cu were insignificantly changed. These UV-ozone-treated Cu NPs showed ~51% Faradaic efficiency of the C2+ conversion (FEC2+) at –0.98 V vs. RHE, which was twice as high as that of the pristine Cu NPs (~25%). In particular, the FEC2+ gradually increased as the remaining capping ligands were removed, indicating the increased catalytic sites for 3 h CO_2RR. In sharp contrast, the FEC2+

from the pristine Cu NPs was consistently low despite the partial stripping of the capping ligands, suggesting the negligible formation of the C2+ active sites. For prolonged chronoamperometry tests for 20 h, these FEC2+ values were retained for both catalysts, while the size and shape of Cu catalysts were differently changed. The UV-ozone-treated ones proceeded little agglomeration and contained many grain boundaries. In contrast, the pristine Cu NPs were transformed to the cubic particles with ~100 nm size. The distinct alternations of Cu structures are closely related to the yield of the C2+ active sites, which I will discuss in this presentation.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 408 (Live Streaming) TUE 10:30

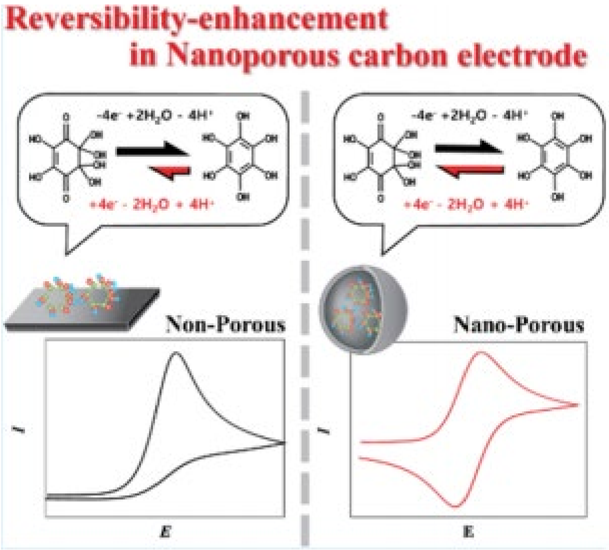
Chair: Chang Hyuck Choi (GIST)

Nano-confinement effects on enhanced reversibility of redox reactions coupled with an irreversible chemical process by electrolysis acceleration in nanoporous carbon electrodes for redox-enhanced electrochemical capacitor

Jaehyun Jeon, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

Redox-enhanced electrochemical capacitors (Redox-ECs) in which electrons are stored and released by redox reactions of organic molecules either dissolved in an electrolyte or adsorbed on an electrode surface represent a promising energy storage system with electrochemical characteristics of both rechargeable batteries and electrical double-layer capacitors. However, the choices for redox-active molecules in Redox-ECs are often limited due to an irreversible nature induced by chemical processes, such as hydrolysis, coupled with e−-transfer reactions. Here, we describe the effects of nanoconfinement on enhanced reversibility in the redox reaction of an electroactive organic molecule undergoing irreversible hydrolysis after e−-transfer in a nanoporous carbon electrode. The redox reaction between hydrated rhodizonic acid (RDZ·$2H_2O$) and hexahydroxybenzene (HHB) via tetrahydroxy-1,4-benzoquinone served as a model in which RDZ is irreversibly hydrolyzed to RDZ·$2H_2O$. This phenomenon results from electrolysis acceleration within confined nanoregimes in a porous carbon matrix, which is analyzed by finite-element analysis. We built asymmetric ECs composed of nanoporous carbon electrodes, one of which was coated with RDZ·$2H_2O$. Due to the enhanced reversibility of the RDZ·$2H_2O$/HHB redox reaction in a nanoporous carbon electrode, Coulombic efficiency of the cell remained near 90% despite the irreversible nature of RDZ via hydrolysis. This research provides fundamental insights into the use of organic molecules in energy storage using redox electrolytes such as Redox-ECs and organic redox flow batteries.


Reversibility-enhancement
in Nanoporous carbon electrode
-4e⁻ +2H₂O - 4H⁺
+4e⁻ - 2H₂O + 4H⁺
HO
OH
O
-4e⁻ +2H₂O - 4H⁺
+4e⁻ - 2H₂O + 4H⁺
Non-Porous
Nano-Porous
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Oral Presentation : **ELEC.O-8**
Oral Presentation of Young Scholars in Electrochemistry
Room 408 (Live Streaming) TUE 10:45
Chair: Chang Hyuck Choi (GIST)

Nanoporous Ta3N5 via Electrochemical Anodization Followed by Nitridation for Solar Water Oxidation

Pran Krisna Das, Soon Hyung Kang[1,*]

Advanced Chemicals & Engineering, Chonnam National University, Bangladesh
[1]*Department of Chemical Education, Chonnam National University, Korea*

Porous tantalum nitride (Ta3N5) is a promising visible-light-driven photoanode for photoelectrochemical (PEC) water splitting with a narrow band gap of approximately 2.0 eV. It can utilize a large portion of the solar spectrum up to 600 nm to improve the activity of photooxidation reactions because of enhanced light scattering and an overall increase of surface area with high light absorption and carrier collection. Herein, we synthesized a new n-type nanoporous tantalum nitride film on Ta foil by an electrochemical anodization in a fluorinated-based electrolyte. Post-annealing in a nitrogen/ammonia mix gas environment then transformed the amorphous TaOx to crystalline Ta3N5. Effects of annealing temperature on microstructure, optical property, and PEC property of samples were then investigated under changeable stoichiometry of Ta and N elements in Ta-based nitride film. Results showed that the film annealed at 1000°C exhibited high crystallinity, high visible light absorption, and a highly conductive interlayer between the substrate, resulting in the highest photocurrent density (JSC) of ~ 0.25 mA/cm2 at 1.23 VRHE in PEC water splitting. In addition, depending on the annealing temperature, it is possible to engineer band alignment in the nanoporous Ta3N5 layer, granting a beneficial charge transfer event.

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

General Student Session

Room 302 (Live Streaming) TUE 09:00

Chair: Sungjun Bae (Konkuk University)

Mercury co-benefits of climate policies on rice mercury concentration and exposure in China

Ju Hyeon Lee, Sae Yun Kwon[*]

Division of Environmental Science & Engineering, Pohang University of Science and Technology, Korea

Atmospheric mercury emissions in China are affected by both international agreements for climate mitigation under the Paris Agreement and mercury controls under the Minamata Convention on Mercury, which may lead to public health benefits for those who consume rice. Rice ingestion is suggested to contribute more to human mercury exposure relative to fish ingestion in China. We combine climate and mercury policies that affect widespread atmospheric mercury emissions from various anthropogenic sectors to measure changes in Chinese rice methylmercury concentrations, exposure and health effects through an integrated model assessment. Our results suggest that rice mercury level is more effectively mitigated by mercury policies relative to climate policies at a national scale. Mercury co-benefits of climate policies, or the mercury mitigation effect of climate policies on rice mercury levels result in less than 1% additional decrease in mercury emissions in China. Provincial-level spatial variations show that central China demonstrates the highest rice production and consumption, and the largest potential public health benefits from mercury policy in China. This suggests significant health benefits to those who are exposed to large amount of mercury via intensive rice consumption in China. However, potential beneficial effects of climate and mercury policies combined are expected to be small in terms of cost-effectiveness relative to mercury policy implementation alone. Mercury-specific policies are more crucial in reducing rice mercury levels in China. Thus, China’s commitment on the Minamata Convention on Mercury is central to reducing rice mercury levels.

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

General Student Session

Room 302 (Live Streaming) TUE 09:20

Chair: Sungjun Bae (Konkuk University)

Enhanced Ammonia Synthesis under Neutral pH Condition using Rh-based Nitrogen Reduction Catalysts

Sunki Chung, Minjun Choi, Kahyun Ham, HyungKuk Ju[1,*], Jaeyoung Lee[*]

School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Korea

[1]CSIRO Energy, Australia, Australia

Ammonia (NH3), one of the important chemicals in the global economy, is generally used for the production of fertilizers, refrigerants and other chemical feedstocks. Ammonia is also being considered as an effective carbon-free energy carrier due to its' high density of hydrogen. Haber-Bosch process which is the main route for ammonia synthesis, requires huge energy consumption. As an alternative route for green ammonia production, electrochemical method for ammonia synthesis at ambient conditions has been recently received much attention. In this study, a molybdenum decorated rhodium electrode (RhMo/C) is fabricated using an electrodeposition technique. With the dual active sites of Mo and Rh for nitrogen reduction reaction (NRR), the RhMo/C electrode shows a higher yield of ammonia and higher faradaic efficiency in comparison with the pristine Rh/C electrode. Moreover, the operation under neutral pH conditions successfully suppressed the hydrogen evolution reaction (HER) which is the competing reaction at the cathode for the electrochemical ammonia synthesis. This study reveals the relationship between the reaction condition and the selectivity of ambient ammonia synthesis.

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

General Student Session

Room 302 (Live Streaming) TUE 09:40

Chair: Sungjun Bae (Konkuk University)

Non-noble Metal Oxygen Evolution Electrocatalyst for Anion Exchange Membrane Water Electrolysis

Sinwoo Kang, Kahyun Ham, Jaeyoung Lee*

School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Korea

We propose corrosion-resistant carbon-coated $Co_{0.9}Fe_{0.1}$ alloy nanoparticles as highly active and durable electrocatalysts for the oxygen evolution reaction (OER) in anion exchange membrane water electrolysis (AEMWE). In the presence of 10% Fe atoms, the oxophilicity of Co metal is modulated in a direction to facilitate OH^- adsorption on Co^{3+}; thus, $Co_{0.9}Fe_{0.1}$-carbon nanofiber (CNF) can exhibit smaller overpotentials than other metal ratios in $Co_{1-x}Fe_x$-CNF. Additionally, we confirm catalytic degradation from the oxidation of the carbon layer, which is triggered by defects in the carbon originating from Fe during the pyrolysis step. The $Co_{0.9}Fe_{0.1}$ metal is further optimized by increasing graphitization to simultaneously achieve superior activity and durability for application on AEMWE. This work not only demonstrates the role of Fe in Co metal for controlling the proper oxophilicity but also shows the importance of graphitized carbon as a catalyst support for stable water oxidation.

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

General Student Session

Room 302 (Live Streaming) TUE 10:00

Chair: Sungjun Bae (Konkuk University)

Assessment of microplastic removal in drinking water treatment process

SangHeon Na, EunJu Kim[1,*]

Division of Energy & Environment Technology, KIST School, Korea

[1]*Center for Water Resource Cycle Research, Korea Institute of Science and Technology, Korea*

The plastic particles smaller than 5 mm, called microplastics (MPs), have aroused increasing concerns in recent years as they can pose various threats to living organisms. The massive use of plastic products and inadequate management of plastic wastes lead to MPs being ubiquitously found in water bodies, including not only oceans but rivers and lakes that are the main drinking water supply sources in Korea. Despite the fact that drinking water is directly relevant to human health, little attention has been paid to the occurrence and fate of MPs in drinking water treatment plants from surface water sources. Under this frame, the present work aims to identify the removal performance of MPs at different stages (coagulation and sand filtration) of the lab-scale drinking water treatment system that derived from the purification of surface waters. We applied polystyrene particles in the size range of 10−90 μm and analyzed their mass with Raman imaging technique to estimate the removal efficiency of MPs.

Poster Presentation : **POLY.P-1**
Polymer Chemistry
Zoom 1 WED 16:30~17:00

Catalysis for ATRP using organic photo-catalysts and visible-light irradiation

Minki Cho, Eunsung Lee[1], Kyung-sun Son[2,*]

Chungnam National University, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*
[2]*Department of Chemistry, Chungnam National University, Korea*

The metal-free atom transfer radical polymerization (ATRP) under visible light irradiation and activated by new organic photo-catalysts (PCs) was investigated. A series of PCs based on N-trifluoromethylphenyl phenoxazine were evaluated for organocatalyzed ATRP (O-ATRP). Especially, 3,7-di(4-biphenyl) 4-trifluoromethylphenyl-10-phenoxazine enabled successful O-ATRP with good catalytic performance, producing well-defined polymers with low dispersity under irradiation with a CFL bulb, white LEDs, or sunlight. With the advantages of visible light catalysis and a metal-free strategy, these organic PCs would further broaden the scope of application of this process.

Poster Presentation : **POLY.P-2**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Alternating ring-opening copolymerization of epoxide and anhydride using a chromium complex with a sterically demanding amino triphenolate ligand

Ho Kyun Ryu, Eunsung Lee[1,*], Kyung-sun Son[2,*]

Chemistry, Chungnam National University, Korea
[1]Department of Chemistry, Pohang University of Science and Technology, Korea
[2]Department of Chemistry, Chungnam National University, Korea

We have investigated alternating ring-opening copolymerization (ROCOP) of epoxides (limonene oxide, cyclohexene oxide) with anhydrides (phthalic anhydride, naphthalic anhydride and maleic anhydride) using a chromium complex containing sterically-demanding amino triphenolate ligand. The polymerization reactions were strongly affected by the type and the amount of co-catalyst, reaction time, and feed ratio of monomers. Under the optimized conditions, the chromium complex produced perfectly alternating polyesters with high molecular weights, high glass-transition temperatures, and low polydispersity. It alsoshowed a very high activity (TOF up to 380 h −1).

Poster Presentation : **POLY.P-3**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Open-to-air RAFT polymerization on surface under ambient conditions

Ji Hoon Lee, Woo Kyung Cho[*], Kyung-sun Son[*]

Department of Chemistry, Chungnam National University, Korea

Oxygen (O_2)-mediated controlled radical polymerization was performed on surface under ambient conditions, enabling on-surface polymer brush growth under open-to-air conditions at room temperature and free of metal contamination. Polymerization of zwitterionic monomers using this O_2-mediated surface-initiated RAFT (O_2-SI-RAFT) polymerization method provided a hydrophilic surface, which exhibited antibiofouling effects. This O_2-SI-RAFT polymerization strategy can avoid prior deoxygenation steps or the use of inert conditions for polymerization, thus it could be applied for the substrates with large surfaces under ambient benchtop conditions, enabling surface functionalization in a practical and user-friendly manner.

Poster Presentation : **POLY.P-4**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Light-Mediated Control of Interfacial Behavior for Thin-Film Block Copolymer Wetting

Sol An, Sangwon Kim[1,*], Myungwoong Kim[*]

Department of Chemistry, Inha University, Korea
[1]*Dept. of Polymer Sci Eng, Inha University, Korea*

In order to achieve spatial control of domain orientations in block copolymer thin films, we designed and synthesized a crosslinkable photosensitive random copolymer, namely poly(styrene-*r*-*ortho*-nitrobenzyl methacrylate-*r*-glycidyl methacrylate) (PSNG). A spin-coated thin film of the random copolymer was thermally crosslinked to create a light-sensitive surface. The extent of deprotection reaction of the *o*-nitrobenzyl group was effectively modulated by adjusting UV light energy irradiated to the crosslinked film. Accordingly, surface energy of the mat was tunable, further enabled the control of domain orientations in overlying lamellar or cylinder-forming poly(styrene-*b*-methyl methacrylate) thin films from perpendicular to parallel depending on UV light dosage. The results were further expanded to the use of photolithography to define the regions of the block copolymer domains with desired orientations.

Poster Presentation : **POLY.P-5**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Cathepsin B-responsive smart liposomes for doxorubicin delivery

Seulgi Lee, Joon Sig Choi*

Department of Biochemistry, Chungnam National University, Korea

In recent decades, many kinds of anticancer drugs that inhibit cancer cell growth and cause cell death have been developed for chemotherapy. However, these agents are associated with side effects due to non-specific delivery, resulting in cytotoxicity to normal cells. To reduce the non-specific delivery of anticancer drugs, nanoparticles have been successfully used for the delivery of anticancer drugs to specific target sites. In this study, a functional polymeric lipid, PEG-GLFG-K(C16)2 (PEG-GLFG), is synthesized to provide cathepsin B enzyme-responsive liposome for controlled anticancer drug delivery. The liposome composed of PEG-GLFG/DOTAP/DPPC/cholesterol was prepared and characterized at various ratios. The GLFG liposome were able to form stable liposome and be degraded by cathepsin B enzyme. Doxorubicin (Dox) loaded GLFG liposome (GLFG/Dox) were found to have an efficient anticancer effect on Hep G2 cells in vitro and inhibited cancer cell proliferation in a zebrafish model.

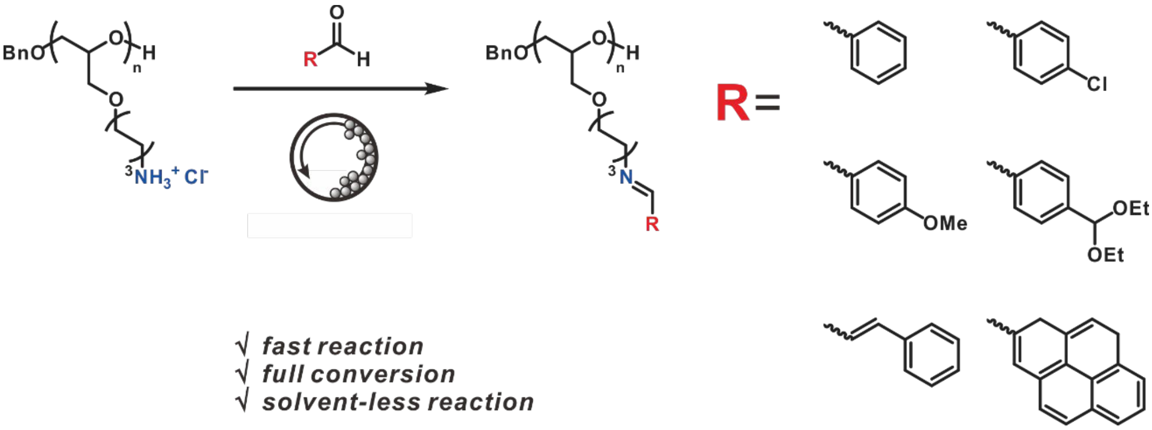
Poster Presentation : **POLY.P-6**
Polymer Chemistry
Zoom 1 WED 16:30~17:00

Mechanochemical Post-Polymerization Modification of Ammonium-Functionalized Polyethers

Joo Won Lee, **Jeung Gon Kim**[1,*], **Byeong-Su Kim**[*]

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

An imine formation is generally achieved by reacting amines and aldehydes in organic solvents. However, ammonium salts are typically insoluble in organic solvents, thereby limiting conventional reaction methods. Alternatively, a solvent-free mechanochemical reaction is an ideal technique for achieving successful imine formation with ammonium salts. Herein, a post-polymerization modification of ammonium-functionalized polyethers is demonstrated by a solvent-free mechanochemical reaction. Polyethers having ammonium pendant groups are prepared by Staudinger reduction of well-defined azide-functionalized polyether. The mechanochemical reaction is performed by vibrational ball-milling technique to afford the fast and efficient formation of imines in pendant groups. The versatility of a wide scope of aldehydes to this approach is evaluated, suggesting this study provides fast and efficient method for the post-polymerization modification of polymers with incompatible molecules in solution.



Poster Presentation : **POLY.P-7**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Improved network formation in polyelectrolyte complex hydrogels via suppression of micellization

Jihoon Han, Younsoo Kim[1],*

Materials Science and Engineering, Pohang University of Science and Technology, Korea

[1]*Department of Materials Science and Engineering, Pohang University of Science and Technology, Korea*

Physical hydrogels composed of oppositely charged polyelectrolytes have unique functions like sol-gel transition and self-healing. However, it is difficult to obtain both of high water content and excellent mechanical properties in the physical hydrogel. Generally, physical hydrogels can be easily obtained by using ABA triblock copolymers, where A blocks are charged blocks and B blocks are hydrophilic neutral blocks. At critical gelation concentration, ABA triblock copolymers construct a 3-dimensional polymer network through self-assembled micelles, especially flower-type micelles. In this case, the loop-shaped polymers do not contribute to connection of network at all, which lowers the efficiency of gel formation. Here, we propose new BABAB pentablock copolymers showing direct network formation rather than loop formation through suppression of micellization. The mechanism of the directly formed polymer network as well as the rheological properties of our hydrogels will be discussed.

Poster Presentation : **POLY.P-8**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Synthesis of Core-Crosslinked Star Polymer via Single Chain Collapse of Graft Copolymer Precursor

Jiyun Nam, Jae suk Lee[1], Myungeun Seo[2,*]

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

[1]Department of Advanced Materials Engineering, Gwangju Institute of Science and Technology, Korea

[2]Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology, Korea

Core-crosslinked star (CCS) polymers containing multiple arms tied to the crosslinked core are typically synthesized by polymerization of a crosslinker in the presence of a macroinitiator. However, the synthesis of well-defined CCS polymers with controlled arm number and crosslinking density has been challenging. Here, we introduce a new synthetic approach by utilizing a well-defined graft copolymer as a precursor to the CCS polymer. To construct the primary structure of star polymer, grafting-through copolymerization of macromonomers with functional monomer possessing crosslinkable group and subsequent single chain collapse produces the target CCS polymer. We anticipate that our methodology will offer a new level of structure control in the CCS architecture.

Poster Presentation : **POLY.P-9**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Fabrication of Cation-π Interacted Graphene Hydrogels for Highly Robust Supercapacitors

Im Kyung Han, Younsoo Kim*

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

Flexible supercapacitors are considerable interest as mobile power supply for future flexible electronics. In this regard, graphene hydrogels are considered promising flexible supercapacitors because they can exhibit both excellent electrical conductivity, flexibility and mechanical robustness. Here, we newly fabricated physically cross linked graphene hydrogels via cation-π interaction with zwitterionic imidazolium based polymers. We established facile and novel synthetic methods for fabricating cation-π interacted graphene hydrogels by using microwave irradiation which induces exfoliation of graphite and polymerization simultaneously.In this presentation, facile method to fabricating graphene hydrogels and their electrochemical performances will be discussed.

Poster Presentation : **POLY.P-10**
Polymer Chemistry
Zoom 1 WED 16:30~17:00

Phase Separated Hydrogels with Embedded Microgels to Improve Shrinking and Re-swelling

Taehun Chung, Younsoo Kim*

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

Thermoresponsive hydrogels have attracted considerable interest in various fields because they undergo volumetric changes in response to temperature. For the application of a versatile thermoresponsive hydrogel, fast swelling/shrinking and large volumetric changes are required. In addition, for repeatable use, the shrunken gel should re-swell rapidly until it reaches an equilibrium swollen state. Here, we propose a novel type of thermoresponsive hydrogels that show improved shrinking and re-swelling. By using globular structure of poly(*N*-isopropylacryamide) in salt solution, it is possible to synthesize phase separated hydrogels with large and rapid shrinkage than normal type of hydrogels. Furthermore, we incorporated simply synthesized microgels in phase separated hydrogels. As a result, hydrophilic and ionic microgels effectively improved the rate of swelling. In this presentation, synthetic strategy of thermoresponsive hydrogels and improved kinetics of them will be discussed.

Poster Presentation : **POLY.P-11**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Fe(III) Assisted Layer-by-Layer Assembly of Pullulan and Tannic acid

Hyunjung Lee, Ji Hun Park[1,*]

Science Education, Ewha Womans University, Korea
[1]*Department of Science Education, Ewha Womans University, Korea*

In this work, we demonstrate layer-by-layer (LBL) assembly of pullulan and tannic acid (TA) with Fe(III). The resulting LbL nanofilms were characterized by spectroscopic ellipsometry for thickness measurement, X-ray photoelectron spectroscopy (XPS) for atomic composition analysis, atomic force microscopy (AFM) for topography analysis, and UV-Vis spectroscopy for nanofilm deposition monitoring. It is to note that a single deposition of Fe(III)-TA layer on Fe(III)-pullulan layer can grow ca. 10 nm-thick Fe(III)-TA nanofilm, which is considerably thicker than the previously reported thickness value of Fe(III)-TA nanofilm deposition (ca. 3 nm). The polysaccharide-polyphenol LBL nanocoating demonstrated herein could be hybridized with diverse nanomaterials including metal nanoparticles and silica nanoparticles for future nanobiotechnological applications, such as smart biosensors, multifunctional protective nanocoatings, and nanotheranostic agents.

Poster Presentation : **POLY.P-12**
Polymer Chemistry
Zoom 1 WED 16:30~17:00

Influence of water absorption on chemical properties of epoxy composites

Hyun Deung Park

Hyundai Motor Group- Hyundai KEFICO, Korea

Metal migration causes dendritic growths and failure in the conductor under conditions conducive to electro-crystallization. Polar liquid medium such as condensed water is present in the path of movement and causes dendritic growths. Epoxy composites have been used as the packaging materials in electronics to prevent this failure.In this paper, the influence of water absorption on the chemical properties of epoxy composites is studied. The conducted samples with various curing conditions (temperature, time) were subjected to water absorption. It is found that the rates of water absorption and initial glass transition were measured depending on the curing temperature and time. The results showed that the higher moisture absorption samples had a lower glass transition temperature and led to more decomposition of chemical structures. During this study, it was possible to establish the optimum process conditions for epoxy composites.

Poster Presentation : **POLY.P-13**
Polymer Chemistry
Zoom 1 WED 16:30~17:00

The Effect of NLS Peptides on Transfection Efficiency of Low Generation PAMAM Dendrimer

Jeil Lee, Younjin Kim, Joon Sig Choi*

Department of Biochemistry, Chungnam National University, Korea

Polyamidoamine (PAMAM) dendrimer is one of the extensively studied polymers in the biomedical research field because of low polydispersity, distinct molecular structure, and surface functionalities. Generally, High generational PAMAM dendrimer is used for gene delivery since transfection efficiency is dependent on charge density. In this study, we selected PAMAM generation 2 to reduce the cytotoxic effect and synthesized RRLHL sequence, nuclear localization signal (NLS) derived from herpesviridae to PAMAM generation 2. The transfection efficiency of RRLHL-PAMAM G2 was like that of polyethylenimine (PEI) in Neuro2A and HT22 cells whereas their transfection efficiency was much higher than the capacity of PEI in Hacat and NIH3T3 cells. Our study shows that low generational PAMAM dendrimer conjugated with NLS sequences has potential as one of the alternatives of PEI in gene delivery.

Poster Presentation : **POLY.P-14**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

High temperature curable and nanoporous substrates for printed electronics

Veasna Soum, Nguyet Mai Ly, Nayoon Pyun, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Printing of nanomaterial inks for printed electronics requires a printing substrate that has glossy surface, absorbing layer, and high temperature curable. Polyether sulfone (PES) thin film, a high-performance substrate for printing nanomaterial inks, was prepared as a free-standing thin film. And it was used to coat on rough surface substrates such as paper and fabric, and unabsorbed layer substrate such as plastic substrate and glass wafer to turn those surfaces have glossy surface and absorbed layer, respectively. The PES film was found to have nanoporous surface and microporous structure in its matrix. They function as a nanomaterial ink-receiving layer and a solvent absorbed layer, respectively. Conductive inks, silver nanoparticle (AgNP), carbon nanotube (CNT), and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) ink were printed on the prepared PES-based substrates using noncontact and contact printing methods. The conductive printed patterns on PES-based substrates showed highly electrically conductive after annealing at high temperature up to 200 ºC, high resolution, and durable. The PES-based substrates show excellent characteristics that are suitable for printed electronic applications.

Poster Presentation : **POLY.P-15**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Effect of circularly polarized light on amplification of supramolecular chirality

<u>Jun Su Kang</u>, Myungeun Seo[1,*]

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

Homochirality in terrestrial life is understood as the results of transfer and amplification of chiral information from a molecular scale to mesoscopic and macroscopic scales. In these evolutionary processes, molecular chirality is considered to dictate direction of supramolecular chirality that amplifies chirality by self-assembly. A few recent examples have reported that supramolecular chirality can be also developed by external stimuli such as circularly polarized light (CPL). Here, we address the effect of CPL in the presence of the small amount of an enantiomer in the evolution of supramolecular chirality. By utilizing light-induced self-assembly of achiral and chiral triphenylamine derivatives as a model system, we will identify the resulting supramolecular helicity and explore contributions of molecular and photonic directors to the chiral amplification in a quantitative manner.

Poster Presentation : **POLY.P-16**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Selective Permeable Polymer Coating on Metal-Organic Framework

Nam Young Ahn, Jooyeon Lee[1], Min Kim[1,*], Myungeun Seo[2,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemistry, Chungbuk National University, Korea*
[2]*Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology, Korea*

Metal-organic frameworks (MOFs) are crystalline microporous materials constructed by coordination bonding of metal ions clusters with multidentate organic ligands. Their high porosity, high specific surface area, and rich metal active sites are anticipated to be useful for catalytic application. The vulnerable coordination bonds against moisture, acid and base, however, intrinsically poses a stability issue. Here we explore coating of individual MOF particles with a porous and permeable polymer shell to improve MOF stability. Synthetic details as well as characterization of mesoporous polymer-MOF composites will be presented.

Poster Presentation : **POLY.P-17**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Development of PEGylated rosmarinic acid liposome for anti-inflammation effect

Seulgi Lee, Joon Sig Choi, Juye Ro[1,*]

Department of Biochemistry, Chungnam National University, Korea
[1]*Chungnam National University, Korea*

Apple mint (Mentha suaveolens) has been used in traditional medicine as a herbal remedy and has a wide range of effects including hypotensive and insecticidal. It shows depressor activity, analgesic, and anti-inflammatory action. Rosmarinic acid (RA) is an active ingredient. It is a water-soluble phenolic compound that is an ester of caffeic acid and 3, 4-dihydroxyphenyl lactic acid. RA has pharmacological effects, such as anti-oxidative, anti-apoptotic, anti-tumorigenic, and anti-inflammatory effects. In this study, we performed encapsulated RA in PEGylated liposomes. And measured physical characterization using DLS, zeta potential, and evaluated the anti-inflammation effect in BV2 cell line. Acknowledgement : This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(2018R1C1B600865313)

Poster Presentation : **POLY.P-18**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Ring-opening copolymerization of cyclic anhydride and epoxide using a chromium complex based on a pentapyridine ligand

Namsik Yu, Ho Kyun Ryu[1], Eunsung Lee[2,*], Kyung-sun Son[3,*]

Department of chemistry, Chungnam National University, Korea
[1]*Chungnam National University, Korea*
[2]*Department of Chemistry, Pohang University of Science and Technology, Korea*
[3]*Department of Chemistry, Chungnam National University, Korea*

This present was study of alternating ring-opening copolymerization (ROCOP) of epoxides (cyclohexene oxide) and anhydrides (phthalic anhydride, naphthalic anhydride) using a novel pentapyridyl Cr(III) complex and cocatalyst (bis(triphenylphosphine)iminium chloride (PPNCl) or 4-dimethyl aminopyridine (DMAP)). The polymerization reaction was affected by the types solvent and cocatalyst. the chromium complex produced fully alternating polyesters (Mn up to 10.4 kDa,ester >99%) with high glass transition temperatures (up to 166 ℃), and low polydispersity ($Đ \leq 1.30$).

Poster Presentation : **POLY.P-19**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

Polyethyleneamine-MoS_2-epoxy composites with improved thermal and mechanical properties

Shahina Riaz, Soo-Jin Park[1,*]

Chemistry, Inha University, Pakistan
[1]Department of Chemistry, Inha University, Korea

AbstractIn this study, single-step branched polyethyleneimine (PEI)-assisted exfoliation of molybdenum sulfide nanosheets (MoS_2-¬-PEI) was carried out. These functionalized MoS_2-PEI nanosheets were employed as toughening agents for epoxy composites. The loadings of nanosheets were kept lower than 1 wt.%. The mechanical and thermal properties, and interfacial interactions of epoxy composites were investigated. The epoxy composites shown ~67% and ~101% enhancements in fracture toughness (K_{IC}) and in fracture energy (G_{IC}) at nanosheets loadings as small as 0.09 wt.% (EP/MoS_2--PEI-0.09), K_{IC} shows direct linear relationship with the surface free energy and is highest at 52 mJ.m−2 for the EP/MoS_2--PEI-0.09 composite. However, the surface free energy values of EP/MoS_2--PEI-0.16 and EP/MoS_2--PEI-1 composites decreased to 48 mJ.m-2 and 45 mJ.m−2. The overall flexural modulus (E) and strength (σ) were not highly responsive to the addition of the MoS_2--PEI nanosheets. Furthermore, the thermal stability and thermomechanical properties of the epoxy composites improved significantly.

Poster Presentation : **POLY.P-20**

Polymer Chemistry

Zoom 1 WED 16:30~17:00

A comparative study on the nanoinclusion effect of MoS_2 nanosheets and MoS_2 quantum dots on the fracture toughness and interfacial properties of epoxy composites.

Shahina Riaz, Soo-Jin Park[1,*]

Chemistry, Inha University, Pakistan
[1]*Department of Chemistry, Inha University, Korea*

The reinforcement effect of molybdenum sulfide (MoS_2) nanosheets on the mechanical properties of epoxy (EP) composites has been extensively studied. However, the effect of MoS_2 quantum dots (MQDs) on the mechanical properties of EP composites has not been reported yet. In this study, we exfoliated bulk MoS_2 into nanosheets (MNS) and MQDs, and use them as reinforcing materials to fabricate a series of high performance EP composites. The MNS and MQDs were dispersed in the EP matrix up to 1 wt. %. The reinforcement effect of MNS and MQDs on the mechanical properties of EP composites was studied in terms of interfacial properties, fracture toughness, and impact strength. Results demonstrated that MQDs remarkably enhance the fracture toughness, flexural strength, modulus, impact strength and interfacial interactions compared to neat epoxy and the one reinforced with MNS.

Poster Presentation : **POLY.P-21**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

WS_2 nanoplatelets: an advanced reinforcement for epoxy composites

Shahina Riaz, Soo-Jin Park[1,*]

Chemistry, Inha University, Pakistan
[1]*Department of Chemistry, Inha University, Korea*

We present a two-dimensional WS_2-based material as a reinforcement additive to produce thermally stable, mechanically strong, and light-weight epoxy (EP) composites. An aqueous melamine solution was used to exfoliate the bulk WS_2 into nanoplatelets while simultaneously functionalizing them to obtain N-WS_2 nanoplatelets. The results demonstrated that the surface free energy of EP composites had been significantly increased after the incorporation of N-WS_2 nanoplatelets into EP matrix and increases with increased loading of N-WS_2 nanoplatelets up to a maximum value of 54.38 $mJ.m^{-2}$ for the composite containing 0.18 wt.% of N-WS_2 nanoplatelets, suggesting stronger interfacial interaction between EP and N-WS_2. The mechanical properties of the EP composites were analyzed and demonstrated 55%, 101%, 44%, and 15% improvements in fracture toughness, fracture energy, flexural strength, and flexural modulus, respectively, for the composite comprising 0.18 wt.% N-WS_2 nanoplatelets.

Poster Presentation : **POLY.P-22**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Surface-initiated RAFT polymerization of methacrylic acid under ambient conditions

Ji Hoon Lee, Seung-yeon Lee[1], Kyung-sun Son*

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

The formation of poly(methacrylic acid) (PMAA), well-known for its swelling behavior on a silicon substrate, provides a hydrophilic and charged surface. Methacrylic acid (MAA) was polymerized through oxygen (O_2)-mediated surface-initiated reversible addition fragmentation chain transfer (SI-RAFT) polymerization under ambient conditions, enabling surface coating with polyelectrolyte brushes. This polymerization strategy enables on-surface polymerization under open-to-air conditions and free of metal contamination, providing an experimenter-friendly method for surface coating using polymers in an easy and convenient way.

Poster Presentation : **POLY.P-23**

Polymer Chemistry

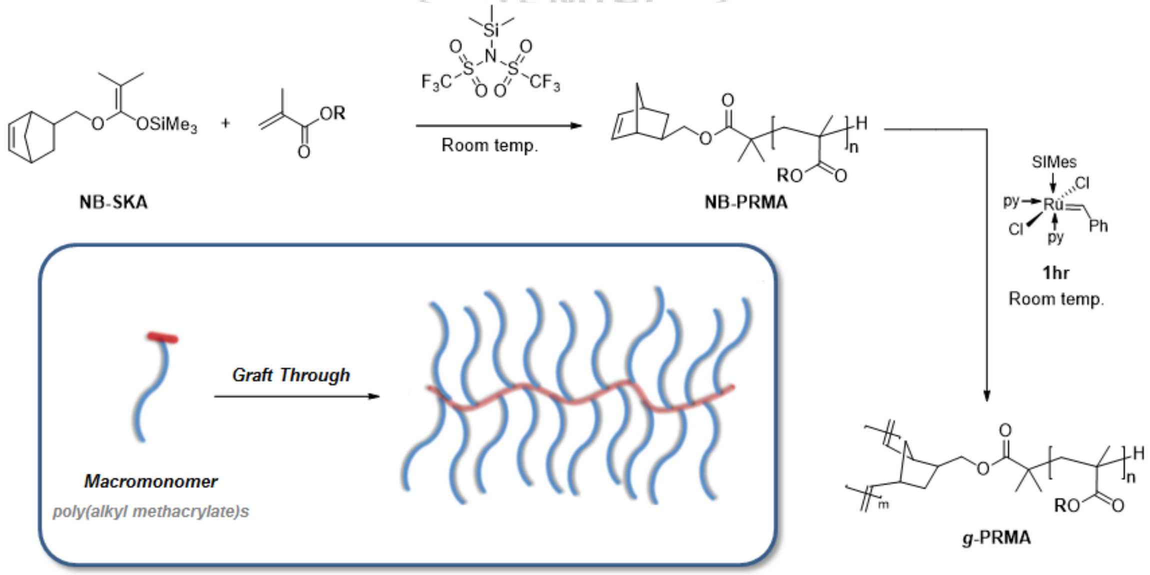
Zoom 1 WED 17:00~17:30

Well-Defined Norbornenyl-Terminated Poly(alkyl methacrylate)s: Their Synthesis by Group Transfer Polymerization and Graft-through Ring-Opening Metathesis Polymerization

Gue Seon Lee, Jeung Gon Kim[1,*]

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

Group Transfer Polymerization (GTP) with controllable catalytic activation permit not only methacrylate polymer synthesis under mild conditions, but also very precise control on distribution. We have sought a new synthetic method development for functional brush polymer synthesis, and decide to scrutinize the synthetic scope and Ring-Opening Metathesis Polymerization (ROMP) activity of GTP-based poly(methacrylate) macromonomers. The polymethacrylate-based brush polymer synthesis using Group Transfer Polymerization has not reported yet. Norbonenyl-terminated poly (alkyl methacrylate) s with narrow Molecular Weight Distribution (MWD) were synthesized by GTP using functional silyl ketene acetal initiator. Norbonenyl-terminated poly (alkyl methacrylate) s synthesized a brush polymer via ROMP.



Poster Presentation : **POLY.P-24**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Burn-In Loss Study in UV-Crosslink of Conjugated Polymers and Nonfullerene Acceptors Using Green Solvent Processing in Ternary Blended Organic Photovoltaics.

Dasol Chung, Junwoo Lee, Hae Un Kim, Taehyun Kim, Dohyun Kim, Taiho Park*

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

Burn-in loss in ternary blended organic photovoltaics (OPVs) manufactured by a UV-crosslinkable semicon-ducting polymer (P2FBTT-Br) and a nonfullerene acceptor (IEICO-4F) using a green solvent process, was studied in this work. 150 seconds of UV irradiation were used to crosslink the synthesized P2FBTT-Br and 2-methylanisole were used to dissolve it with its asymmetric structure. In OPV test for performance and burn-in loss 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 devices. The anchored morphology from the crosslinking prohibits lateral crystallization and aggregation leading to morphological degradation. When IEICO-4F was introduced as a substitute for the fullerene-based acceptor, the burn-in loss brought by the temperature and light was effectively suppressed due to the anchored morphology and high miscibility of the nonfullerene 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), the highest value in crosslinked active materials using the green processing approach.

Poster Presentation : **POLY.P-25**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Oil/water interface stabilized by amphiphilic heteroarm core cross-linked star polymer

Yunji Jung, Myungeun Seo[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1] *Graduate School of Nano Science Technology, Chemistry, Korea*

A polymer containing hydrophilic and hydrophobic polymer arms extending from the cross-linked core is called an amphiphilic heteroarm core cross-linked star (CCS) polymer. If the constituting arms are intramolecularly segregated, the polymer is expected to effectively stabilize the oil/water interface because of large energetic penalty for desorption from the interface. To prove this hypothesis, we synthesized amphiphilic heteroarm CCS polymer by an “in-out” method based on reversible addition-fragmentation chain transfer (RAFT) polymerization. Synthesis, morphology, self-assembly behavior, and interfacial properties of amphiphilic heteroarm CCS polymer will be discussed in detail.

Poster Presentation : **POLY.P-26**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Synthesis of Functional Polyethylene Block Copolymers via Post-polymerization Deoxygenation

Taeseok Oh, Myungeun Seo[1,*]

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

Polyethylene (PE) is the most used plastic in the world. As an aliphatic polyhydrocarbon lacking heteroatoms, PE inherently holds poor compatibility and adhesion. Copolymerization of ethylene with polar functional monomers has been mostly based on high-pressure radical copolymerization, and synthesis of functional PE with well-defined architectures has been challenging. We suggest a route to functional PE block copolymers via catalytic post-polymerization deoxygenation as a distinct approach from conventional functionalization. Starting with well-defined poly(vinyl acetate) (PVAc) obtained by RAFT polymerization and containing 100% functionality appended by C-O bonds, cleaving it leads to PE. We will demonstrate synthesis of PE-*b*-PS from PVAc-*b*-PS, can be successfully converted into PE-*b*-PS with control of functionalization.

Poster Presentation : **POLY.P-27**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Multiblock Copolymerization-induced self-assembly

Suchan Cho, Myungeun Seo[1,*]

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[1]Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology, Korea

Proteins are known to undergo cotranslational folding during the synthesis to form the unique 3D globular structure and function properly as dictated by the shape. Polymerization-induced self-assembly (PISA) is a block copolymer-based synthetic methodology that mimics the in-situ folding process. Driven by incompatibility of the growing polymer chain to the environments (i.e., solvent), block copolymer micelles form spontaneously. Here we explore multiple chain extension in PISA via reversible addition-fragmentation chain transfer polymerization to produce multiblock copolymers, which can undergo sequence-dependent folding and access complex core-shell morphology.

Poster Presentation : **POLY.P-28**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

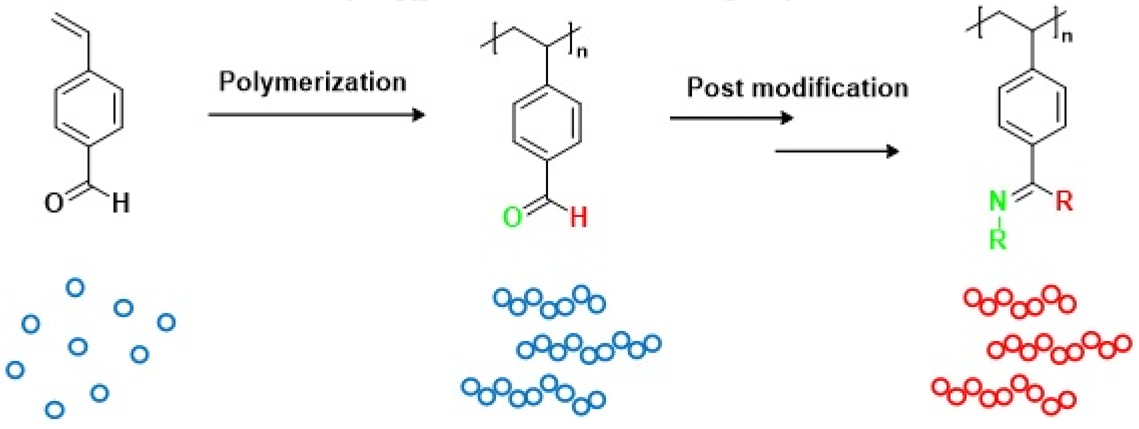
Post-polymerization modification of aldehyde polymers: functionalization of aldehyde polymers

HyoWon Lee, Jeung Gon Kim[1,*]

chemistry department, Jeonbuk National University, Korea

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

Carbonyl group is an important functional group that can be converted into various functional groups. So, we synthesized a polymer with a carbonyl group and conducted a study to convert the other functional group through post-modification polymerization. first, we synthesized a polymer containing aldehyde from 4-Vinylbenzaldehyde (4-VBA) and then successfully converted the aldehyde to ketone through hydroaclylation using the Rh catalyst. In the case of hydroacylation, it was confirmed that polydispersity increased due to the coupling reaction between aldehydes.In addition, in the case of a polymer containing a ketone, it was successfully converted into imine or oxime by reacted with amines. Details of the experiment will be discussed in the poster presentation session.



Poster Presentation : **POLY.P-29**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Preparation of porous polymeric particles by γ-ray radiation and solvent extraction

Yoolee Lee, Daewon Sohn*

Department of Chemistry, Hanyang University, Korea

Porous polymer particles have attracted great interests as they have been applied in numerous ways in many areas of advanced materials science. This research introduces preparation of the porous polymeric particles by γ-ray radiation and solvent extraction. The sodium poly(styrene sulfonate) emulsions are formed in the hexadecane with surfactant. Inverse emulsion polymerization format with surfactant method is used to form water in oil (w/o) emulsions. So, polymeric particles have been fabricated by γ-ray induced crosslinking of polystyrene sulfonate and the pores are formed by methyl ethyl ketone (MEK) which extracts the water within the polymer particles because MEK is miscible in both organic solvents and water. The concentration of sulfonyl groups in the particles contributed to the amount of absorbed MMA and water, leading to various pore and particle sizes. It was possible to flexibly manipulate the inner space using non-grafted PS particles. Since PMMA served to strengthen PS, a porous structure was maintained when MMA was polymerized into PMMA via gamma ray irradiation. The synthesized porous particles could be used in various applications such as heat insulating material and adsorbents.

Poster Presentation : **POLY.P-30**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Electropolymerization of thiophene and selenophene derivatives and their application in capacitors.

Eunsang Yu, Intae Kim*, Yang-Rae Kim*

Department of Chemistry, Kwangwoon University, Korea

Three kinds of thiophene and selenophene-based monomers were synthesized through a Stille cross-coupling reaction. The compounds were analyzed by proton nuclear magnetic resonance, carbon nuclear magnetic resonance, and mass spectrometry. The electropolymerization processes of these monomers were carried out on glassy carbon and gold electrodes. And the electropolymerization process and electrochemical characterization of deposited polymer layers for anion intercalation were performed by cyclic voltammetry and electrochemical quartz microbalance techniques. Through the intensive studies, it was confirmed that the anion intercalation processes into the deposited polymer layers under various applied potentials are dependent on the structure of monomers and the kinds of anions. As a result, the performances for electrochemical stability and capacitance of the deposited polymer layers were investigated.key words : Electropolymerization, Chalcogen group, Thiophene, Selenophene

Poster Presentation : **POLY.P-31**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Fabrication of acrylic based polymer resin for Thermochromic material

Munseok Choi, Hoyoul Kong*

Korea Research Institute of Chemical Technology, Korea

Among various physical stimuli, temperature is difficult to detect visually. Therefore, it is important to develop real-time sensitive materials which change color appearance due to temperature change.Recently, research on various visualization techniques for temperature stimulation has been conducted. Specifically due to its simplicity and lack of separate stimuli, paint that changes color in real time due to temperature change is the common one.In this study, we made acrylic polymers that can be used as binders in temperature sensitive paints. The physical properties of acrylic polymer structure were analyzed, and additionally the optimal conditions were established by comparing binder properties suitable for paint.

Poster Presentation : **POLY.P-32**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Formulation of Nanocomposite Hydrogel for Heat Responsive Waterless Soft Actuator

Monica cahyaning Ratri, Veasna Soum, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Soft actuator, a bio-inspired mimicking system, is the one of strategy in the medical, soft robotic, pharmaceutical, and tissue engineering due to its dynamic movement toward the presence of external stimuli. The 3D printed object offers sophisticated and innovative functions such as jumping, complex 3D movement, gripping and releasing by enhancing the additive manufacturing technique and material synthesis. A combination of different formulation of ink, such as active and passive material, can be harnessed to initiate the soft actuator movement expectedly. Poly (N-isopropyl acrylamide) (PNIPAAm) is one of the well-known as active polymers that have temperature-sensitive property, shrinking above its lower critical solution temperature (LCST) and swelling below LCST. As a passive material, Poly-acrylamide (AAm) combined with alginate has high toughness and elasticity. Due to its surface plasmon resonances (SPR) properties, gold nanorods can absorb light and release heat to its surrounding. Therefore, the nanoparticle's illumination with Near Infrared (NIR) can generate heat locally and initiate the heat-induced actuation to PNIPAAm containing matrices. The irradiation of the NIR lamp had been done outside the water. The waterless actuation process is one of the advantages of this system. We formulated and tested PNIPAAm-metal nanoparticle composites as an ink material to fabricate the heat-sensitive soft actuators for photo-responsive soft robotic motions. We will present our preliminary results to formulate the nano-composite ink and photo-responsive reactions of the 3D printed soft actuators.Keywords: Waterless soft actuator, PNIPAAm, Gold nanorods

Poster Presentation : **POLY.P-33**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Development of hydrogel based lateral flow diagnostic devices

Nayoon Pyun, Kwanwoo Shin[1,*], Oh-Sun Kwon[1], Nguyet Mai Ly[1], Veasna Soum[1]

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

Recently, major public health issues are requiring to develop the point-of care detection devices that can be measured quickly and precisely. Conventional paper-based devices, such as strip or lateral flow assays have been extensively studied for a rapid diagnosis using immune responses with colorimetric detections, because of their simplicity, cost-effectiveness, and quick and simple operation. Cellulose as the major constituent of paper, is chemically inert, so paper substrates are lacking in their ability to provide various chemistry for the immobilization of biomacromolecules and control fluid flow. On the other hand, hydrogels made of various synthetic polymers have advantages in controlling the size of pores and varying chemistry through a chemical grafting to cross-linkable monomers. In this research, we intend to manufacture a new concept of lateral flow assay kit that can be controlled in the fluidic flow by coating of various types of hydrogels on a substrate. Moreover, by introducing various binding sites to the hydrogel, various antigens and antibodies can be selectively immobilized.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Zr(IV) Coordination Chemistry for Antiplatelet Alginate Coatings: The Effect of Surface Functional Groups

Yeonwoo Jeong, Sung Min Kang[*]

Department of Chemistry, Chungbuk National University, Korea

Preventing platelet adhesion on artificial surfaces has been of great interest because non-specific adhesion of platelet on solid surfaces triggered biomedical devices to malfunction. To avoid these problems, alginate (Alg) coating has been widely used. However, previous approaches for Alg coating showed several drawbacks: (i) derivatization of Alg is typically also required and (ii) these methods only function under specific reaction conditions. Herein, we demonstrate efficient Alg grafting onto carboxyl-, catechol-, polydopamine-, and tannic acid-functionalized surfaces via Zr(IV)-mediated cross-linking reactions. Alg multilayers constructed by this strategy successfully suppress platelet adhesion onto the solid surfaces. Given its ease of use and the wide selection of available carboxyl polymers, the current strategy is expected to be a useful tool for preparing functional polymer films for various applications.

Poster Presentation : **POLY.P-35**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Surface/interface controls of piezo-resistive flexible pressure sensors for improving linearity and robustness

Hyeon Ju Ko, Seung Goo Lee*

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A piezo-resistive type pressure sensor with high stretchability and linear sensitivity was developed via the in-situ formation of nano-cracks and micro-wrinkles on pyramidal elastomers using the tensile/compressive residual stress applied on metal thin film. The nano-cracks generated in the process of thermal evaporation improved the stretchability, and the micro-wrinkles formed during the deformation of pyramidal structure helped to achieve the linear sensitivity. Furthermore, our pressure sensor maintained its sensing performance even after repeated pressure cycle tests due to high interfacial adhesion between the surface thiolated elastomer and the deposited metal thin film.

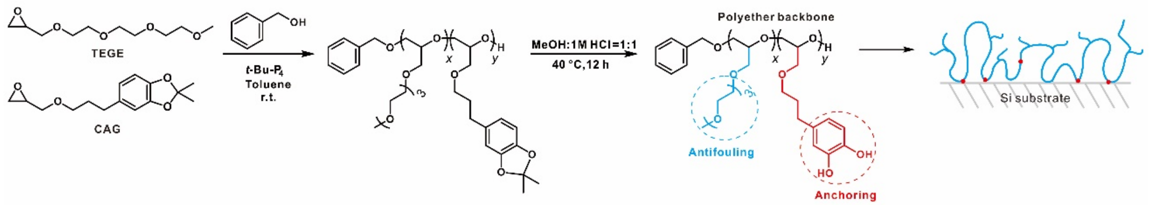
Poster Presentation : **POLY.P-36**
Polymer Chemistry
Zoom 1 WED 17:00~17:30

Antifouling Multi-Loop Copolyethers

Suebin Park, Minseong Kim[1], Byeong-Su Kim[*]

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

Poly(ethylene glycol)(PEG) and its derivatives have been widely used for antifouling materials because of their intrinsic lubrication and high level of hydration. While coatings using PEG brushes are widely used, recent work suggested the enhanced antifouling effect of different topology such as polymeric loops owing to their large excluded volume, and strong steric hindrance. In this study, we explored the effect loop dimension within the framework of multi-loop copolymers. In particular, we designed and synthesized functional epoxide monomers, including triethylene glycol glycidyl ether (TEGE) and catechol-acetonide glycidyl ether (CAG), to afford the poly(TEGE-*co*-CAG)$_n$ via anionic-ring opening polymerization. Specifically, TEGE was designed as a short PEG segment for antifouling effect and CAG was used as a mussel-inspired moiety for surface coatings. It was found that the deprotected CAG moiety facilitated the anchoring of the poly(TEGE-*co*-CAG)$_n$ on various surfaces, while leaving the TEGE moiety with varying sizes of loops. The successful antifouling could be evaluated depending on the loop size using various characterizations.



Poster Presentation : **POLY.P-37**
Polymer Chemistry
Zoom 1 WED 17:00~17:30

Grafting of poly(acrylic acid) from silica particles in gelation process

Jungju Ryu, **Daewon Sohn***

Department of Chemistry, Hanyang University, Korea

Particle-induced polymer networks have attracted great attention in wide area of environmental, industrial, and biomedical application, due to the facile method to achieve better properties in mechanical strength and functionality. Thus, there have been a lot of efforts to reveal gelation mechanisms of the particle-induced polymer networks. However, these investigations have focused on the overall characteristics of networks, and the details about particle behaviors have not been addressed. Here, we explored behaviors of particles that provide a platform of polymer grafts, upon gelation time evolution, in order to know how they make networks. We prepared silica-poly(acrylic acid) hydrogels by introducing gamma-ray treated silica particles, which have roles of crosslinker and initiator. The gelation steps and structural characteristics were investigated by using dynamic light scattering and small angle neutron scattering measurements. We observed the incipient gels have two phases consisting of long-range connections and aggregates of dense clusters, and also revealed the grafting magnitudes of polymer chains are irregular at the initial stages. When the system was close to the gel threshold, three dimensional networks appeared, and the dynamics of the system became relatively homogeneous. Based on the observations, we presented the method to attain silica-poly(acrylic acid) core-shell particles. Consequently, this study provides the details about the silica particles in gelation and effective strategies to develop advanced materials.

Poster Presentation : **POLY.P-38**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Main Chain Conjugated Copolymer Having Donor-Acceptor Heterojunctions for Versatile Outdoor and Indoor Photovoltaic Power Generation

Nayeon Kwon, Su Hong Park, Hun Gu Kang, Young Un Kim, Hyung Jong Kim, Jinhyo Hwang, Hyo Jae Yoon, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

We successfully synthesized a crystalline main chain conjugated copolymer, P(BDBT-co-NDI2T), having BDBT donor-NDI2T acceptor heterojunctions in film states. Interestingly, the polymer exhibited a strong absorption band from 500 to 650 nm, which is overlapped well with the emission spectrum of white light-emitting diodes (LED) used as an indoor light source. The P(BDBT-co-NDI2T) films showed the relatively smooth surface and internal morphology compared to the blend films of P(BDBT) and P(NDI2T). In particular, the Kelvin probe force microscopy data explained the increased uniformity in the distribution of the surface charge in the annealed P(BDBT-co-NDI2T) films as compared to those of the annealed blend films of P(BDBT) and P(NDI2T). Indoor photovoltaics (IPV) produced by using the P(BDBT-co-NDI2T) synthesized in this study as an active layer, showed a high power conversion efficiency of 12.70% (@500 lux) with a short circuit current density of 49.89 □A cm-2. The PCE of the P(BDBT-co-NDI2T) film-based IPV was twice as high as that of the blend film-based IPV and showed excellent operational stability. This study is the first time that the P(BDBT-co-NDI2T) has been applied to IPV, which suggests the potential for their widespread use in the development of indoor organic PVs in the future.

Poster Presentation : **POLY.P-39**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

High Performance Solution-Processable Thermally Activated Delayed Fluorescent OLEDs with Organoboron Acceptor Monomer in Copolymer Host Materials

Jinhyo Hwang, Hyung Jong Kim, Young Un Kim, Nayeon Kwon, Chai Won Kim, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

In particular, polymer hosts in organic light emitting diodes (OLED) have superior characteristics, including facile functionality to introduce various electron donor and acceptor entities, and ability to uniformly disperse and contain small molecular dopants. In this study, we designed and developed three new styrene-based copolymers (ABP91, ABP73, and ABP55) bearing 2,12-di-tert-butyl-7-phenyl-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracene as the electron acceptor and diphenylacridine as the electron donor. In particular, ABP91, ABP73, and ABP55 were synthesized via variations in the ratio of donor to acceptor monomers to substantiate their influence in OLED applications. Consequently, solution-processable OLEDs fabricated using the newly synthesized copolymers as host materials and the familiar t4CzIPN as a green emissive TADF dopant deliver state-of-the-art performance, with maximum EQEs of 21.8, 22.2, and 19.7% for ABP91, ABP73, and ABP55, respectively. To our knowledge, this is the best performance reported when organic polymers are used as host materials in solution-processable TADF OLEDs. The pragmatic outcomes obtained in this study can provide useful insights into the structure–property relationship to the OLED community for the further development of efficient polymer hosts for use in solution-processable TADF OLEDs.

Poster Presentation : **POLY.P-40**

Polymer Chemistry

Zoom 1 WED 17:00~17:30

Flexible Polymer Solar Cells based on Sandwich Type Silver Nanowire Electrodes Between PEDOT:PSS Layers

Young un Kim, Nayeon Kwon, Su Hong Park, Chai Won Kim, Jinhyo Hwang, Hyung Jong Kim, Dong Hoon Choi*

Department of Chemistry, Korea University, Korea

The most widely used transparent electrode material for optoelectronic devices is indium tin oxide (ITO) due to its low sheet resistance but, its high cost, stiffness, and lack of adhesion to organic and polymeric materials make it unsuitable for manufacturing flexible devices on plastic substrates. Therefore, new alternative ductile electrode materials must be developed and AgNW is one of those that meet the requirements.In this study, a simple and effective solution process method for manufacturing AgNWs-based sandwich type flexible transparent electrode is developed and presented. First, a PEDOT:PSS layer was applied to the PEN substrate and AgNWs were applied on it. Finally, to smooth out the rough surface of AgNWs, PEDOT:PSS with high conductivity was coated once again (PEDOT:PSS/AgNWs/PEDOT:PSS). This method was able to dramatically improve the surface roughness of AgNWs electrodes without significant reduction of conductivity. This selective multilayer sandwich type electrode showed a low sheet resistance of 22 Ω/sq, and the transmittance was measured at a maximum of 82%. A three-layer sandwich type electrode was used as an anode for a polymer solar cell (PSC). PSCs with the above electrodes showed similar performance to devices based on ITO anode.

Poster Presentation : **IND.P-41**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Development of Technology for Recovering Valuable Metals in Detoxified Waste Asbestos-Containing Waste

Dong Nyeon Kim, Donghyeon Yang[1], Seok-Chan Kim*

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[1]*chemistry, Kookmin University, Korea*

Asbestos is an inorganic complex composed largely of silicon, magnesium and calcium, and has been used in various industries including building materials due to its outstanding physical and chemical properties. However, since the fatal toxicity to the human body was known, it has been designated as a first-class carcinogen by the World Health Organization (WHO) and is now banned from exporting, importing and using it in most countries. Currently, a large amount of asbestos waste is naturally generated due to the use of various materials replacing asbestos and secondary damage caused by dust, so most of them are buried and disposed of. But landfills are causing soil pollution, and landfill costs are increasing year by year. Therefore, technology development has been carried out to treat asbestos as general waste by heat treatment, and is currently expected to be commercialized. However, despite its harmless treatment, asbestos waste is mostly buried due to a lack of processing space. As a result, the development of technology to deal with it is required.In Korea, few studies have been conducted to recycle asbestos into resources. Therefore, by using waste asbestos, magnesium, silicon, and calcium, the main component metals, were reused through high purity extraction and separation, future environmentally friendly, economical and resource-recycling techniques were developed, and the separated compounds were analyzed through XRD and ICP.

Poster Presentation : **IND.P-42**

Industrial Chemistry

Zoom 1 WED 17:30~18:00

The Substituent-Effect of Deep-Blue Phosphorescent N-Heterocyclic Carbene (NHC) Ir(III) Complexes and The Application in OLED Devices

Changhyun Back, Su-Won Na, Daehan Lee, Sang Ook Kang, Ho-Jin Son[*]

Department of Advanced Materials Chemistry, Korea University, Korea

To evaluate the efficacy of ortho-aryllation in the second coordination sphere of octrahedral iridium complex, a series of homoleptic NHC-based $\mathbf{Ir(C^{\wedge}C^{R})_{3}}$-type complexes were desgined and prepared by introducing various substituents (R = H, Me, Ph, MePh, and diMePh) at the ortho-position of the aryl unit of orthometalling phenyl group. In solution, unnoticiable increase of emission quantum yields was observed within the variation of the ortho-substituent of sterically demanding side-branch, a -diMePh group, showing the radiative quantum yield of ***m*-**$\mathbf{Ir(C^{\wedge}C^{diMePh})_{3}}$ (ΦPL = 1.9%) being higher than that of the pristine carbene-based ***m*-**$\mathbf{Ir(C^{\wedge}C^{H})_{3}}$ (ΦPL = 1.2%).

Poster Presentation : **IND.P-43**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Influence of bulky substituents on the photophysical properties of homoleptic iridium(III) complexes

Su-Won Na, Changhyun Back, Daehan Lee, Dae won Cho, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A new series of homoleptic cyclometalated iridium(III) complexes based on a phenylpyridine (ppy) ligand containing bulky substituents have been synthesized and characterized. The phosphorescence behavior of the Ir complexes is investigated by steady-state and time-resolved emission spectroscopic techniques. Comparison of the results with those of the reference **Ir(ppy)$_3$** reveals that the emission color and photophysical properties of other Ir complexes are influenced by the electron-donating groups (–CH_3 and phenyl derivatives) attached to the ppy ligand. In particular, systematic red-shifts are observed by increasing the electron-donating ability. The emission spectrum of **Ir(Me-ppy)$_3$**, having a small electron-donating –CH_3 group, is red-shifted; however, the emission quantum yield is low and the nonradiative decay constant is large. On the other hand, although bulky phenyl derivative-adducts (**Ir(Ph-ppy)$_3$**, **Ir(MePh-ppy)$_3$**, and **Ir(diMePh-ppy)$_3$**) also exhibit red-shifted emission, their kinetic and photophysical behaviors are more optimal than those of **Ir(Me-ppy)$_3$**, whose behavior does not follow the energy gap law. This deviation may be attributed to the orthogonal structure associated with the steric hindrance of bulky substituents. The molecular structure, molecular orbitals in singlet/triplet manifolds, and energy band gap are verified by density functional theory calculations.

Poster Presentation : **IND.P-44**

Industrial Chemistry

Zoom 1 WED 17:30~18:00

Photophysical properties of structural isomers of homoleptic Ir-complexes derived from xylenyl-substituted N-heterocyclic carbene ligands

<u>Su-Won Na</u>, Changhyun Back, Min Su Choe, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

We investigated the photophysical 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-(2',6'-dimethylbiphenyl-2-yl)-3-methyl-2,3-dihydro-1H-imidazo[4,5-*b*]pyridine). 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 it may be attributed to the fast migration of localization of excited state via intra-ligand energy transfer. An electron density displacement takes place in the excited state accompany with the geometrical change of the dimethylphenyl substituent. Actually, **Ir(dmpmp)$_3$** showed a strong rigidochromic shift in the emission spectra with varying temperature.

Poster Presentation : **IND.P-45**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Facile preparation of starch-based activated carbons for methane storage

Jong-Hoon Lee, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

Methane has attracted attention as alternative fuel because of environmental problems. Methane gas has various attractive advantages such as abundance of resources and lower carbon emissions resulting from a low carbon/hydrogen ratio. For practical energy utilization, efficient storage materials of alternative fuel are essential. There are various types of adsorption materials studied for gas storage. Activated carbons are one of candidate of good methane storage materials due to their good chemical and thermal stability, high porosity, and high methane uptakes. In this work, starch-based activated carbons were prepared by chemical activation process. Carbon materials were prepared at 900 ºC, 1hr, and N_2 flow conditions. The influence of activation reagent ratios was investigated by experience of activated carbons/chemical reagents mass ratio. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The N_2 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). Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

Poster Presentation : **IND.P-46**

Industrial Chemistry

Zoom 1 WED 17:30~18:00

A Effect of TiO_2/reduced graphene oxide composites Prepared by hydrothermal for photocatalytic degradation

Seong-Jun Mun, Soo-Jin Park[1,*]

Inha University, Korea

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Composites consisting of TiO_2/ reduced graphene oxide were synthesized via hydrothermal method. Structural properties of the composites were characterized by X-ray diffraction spectroscopy (XRD) and transmission electron microscopy (TEM). The surface areas and pore size distributions were calculated by Brunauer-Emmett-Teller (BET). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of TiO_2/ reduced graphene oxide composites were improved compared to pure TiO_2. The results indicated that reduced graphene oxide reduced band gap energy and decreased recombination ratio of excited electrons.

Poster Presentation : **IND.P-47**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

A study on polysaccharide based porous carbons for high-pressure methane adsorption

Jong-Hoon Lee, Soo-Jin Park[*]

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In this work, porous carbons (PC) with high specific surface area were synthesized by polysaccharide which produced by abundant biomass. Carbon materials were prepared at 900℃, 1h, and N_2 flow conditions using chitosan as precursor. After carbonized, PC was synthesized by chemical activation. The effect of quantity of activation reagents was investigated by experience of PC/chemical reagent mass ratio. The structure information of the activated carbons was measured by X-ray diffraction (XRD) patterns. The N_2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. The morphology of prepared material was observed using scanning electron microscopy (SEM). Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

Poster Presentation : **IND.P-48**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Preparation and characterization of porous carbons *via* hydrothermal synthesis for gas adsorption

Jong-Hoon Lee, **Soo-Jin Park**[*]

Department of Chemistry, Inha University, Korea

In this work, porous carbons (PC) with high specific surface area were synthesized by hydrothermal method. Carbon materials were prepared at 900°C, 1h, and N_2 flow conditions using chitosan as precursor. After carbonized, PC was synthesized by chemical activation. The structure information of the activated carbons was measured by X-ray diffraction (XRD) patterns. The N_2 adsorption-desorption isotherms were measured at 77 K and calculated by Brunauer-Emmett-Teller (BET) equation. The morphology of prepared material was observed using scanning electron microscopy (SEM). Methane storage capacity was evaluated with a Model BEL-HP instrument (BEL Co., Ltd., Japan) at 298 K and 35 bar.

Poster Presentation : **IND.P-49**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Fabrication of TiO_2/g-C_3N_4 nanocomposites for photocatalytic degradation of RhB

Seong-Jun Mun, **Soo-Jin Park**[1,*]

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

In this work, TiO_2 were prepared by hydrothermal and various weight ratio of g-C_3N_4 composites for photocatalytic activities. Structural properties of the composites were characterized by X-ray diffraction spectroscopy (XRD) and transmission electron microscopy (TEM). The surface areas and pore size distributions were calculated by Brunauer-Emmett-Teller (BET). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of TiO_2/g-C_3N_4 composites were improved compared to pure TiO_2. The results indicated that g-C_3N_4 reduced band gap energy and decreased recombination ratio of excited electrons.Keywords: Photocatalyst, Titanium dioxide, Rhodamine B

Poster Presentation : **IND.P-50**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Fabrication of N-doped TiO_2 nanotubes/reduced graphene oxide nanocomposites for photocatalytic activity

Seong-Jun Mun, **Soo-Jin Park**[1,*]

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

In this work, N-doped TiO_2 nanotubes were prepared by hydrothermal and various weight ratio of reduced graphene oxide composites by hydrothermal method for photocatalytic activities. Structural properties of the composites were characterized by X-ray diffraction transmission electron microscopy (TEM) and spectroscopy (XRD). The surface areas and pore size distributions were calculated by Brunauer-Emmett-Teller (BET). Photocatalytic activities were measured using rhodamine B solution under simulated solar light irradiation. Photodecomposition rate of N-doped TiO_2 nanotubes/reduced graphene oxide composites were improved compared to pure TiO_2. The results indicated that reduced graphene oxide reduced band gap energy and decreased recombination ratio of excited electrons.

Poster Presentation : **IND.P-51**

Industrial Chemistry

Zoom 1 WED 17:30~18:00

Effect of tetraethylenepentamine-impregnated zeolite templated carbon for CO_2 capture

Choong-Hee Kim, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

Zeolite-templated carbons (ZTCs), which have high specific surface area, were prepared by a conventional templating method using microporous zeolite for CO_2 capture. The ZTCs were synthesized at different temperatures to investigate the characteristics of the surface produced. ZTCs were amine modified using tetraethylenepentamine (TEPA) to enhance its properties rather than existing template carbons. The surface properties of the ZTCs characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). The specific surface area and pore size distribution were calculated by N_2 / 77K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). As a result, TEPA on ZTCs lead to improvement of CO_2 absorption behavior.

Poster Presentation : **IND.P-52**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

A study of activated carbons from Pine cones for CO_2 capture

Choong-Hee Kim, **Soo-Jin Park***

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In this work, pine cones activated carbons (PCs) were fabricated using chemical activation with potassium hydroxide (KOH) at different activation temperature. The surface properties of the PCs characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). The specific surface area and pore size distribution were calculated by N_2 / 77K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). As a result, pine cones different activated temperature with CO_2 capture.

Poster Presentation : **IND.P-53**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Development of Stable and Reproducible Liposome Formation for Diacetylene Derivatives via Continuous-Flow Methods

Se Won Bae

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Polydiacetylene, which changes color and fluorescence intensity through photo-irradiation after making liposomes using diacetylene derivatives, has been widely used recently as a chemical sensor. In general, a method of forming liposomes from diacetylene is obtained by forming a thin diacetylene film on the surface of a substrate, injecting distilled water, and applying sonication for a certain period of time while increasing the temperature. However, in this method, the degree of the dieacetylene monomer formed as a liposome is different for each batch, and as a result, the reproducibility of the absorbance intensity or fluorescence intensity of the polydieacetylene formed after photo-irradiation is poor.We set the stability and reproducibility of diacetylene liposomes as an important factor that can be ultimately applied to actual chemical sensor production by improving the automated manufacturing and quality control capabilities of chemical sensors using polydiacetylene. In order to increase the stability and reproducibility of diacetylene liposomes, a new method was developed to form liposomes by injecting a monomer and a buffer in a continuous flow through a microfluidic tube. This method is expected to be widely used in the development and practical use of chemical sensors utilizing polydiacetylene in the future.

Poster Presentation : **IND.P-54**

Industrial Chemistry

Zoom 1 WED 17:30~18:00

Preparation and characterization of activated carbons derived from coffee wastes for hydrogen storage

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[1]Department of Chemistry, Inha University, Korea

In this work, activated carbons (ACs) were fabricated using chemical activation with potassium hydroxide (KOH) at different temperatures. The structural properties and the morphologies of ACs were observed by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The specific surface area and pore size distribution were obtained by N_2/77K adsorption-desorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen uptakes were measured by an adsorption instrument at 77 K and 1 bar. The results present that the different activation temperatures for preparing activated carbons have effects on their porosity with hydrogen storage capacity.

Poster Presentation : **IND.P-55**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Effect of cigarette filters-derived activated carbons on enhanced hydrogen storage

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

In this work, activated carbons (ACs) derived from cigarette filters were prepared by chemical activation with KOH. The morphologies of ACs were investigated by scanning electron microscopy (SEM). The structural properties were investigated by recording X-ray diffraction (XRD) patterns. The specific surface area and pore size distribution were calculated by N_2/77K adsorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen uptakes were evaluated by a gas adsorption instrument at 77 K and 1 bar.

Poster Presentation : **IND.P-56**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

The effective pore sizes of activated carbons from biomass materials for high-pressure hydrogen storage

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In this work, activated carbons (ACs) were fabricated using chemical activation with silica removal step. The structural properties were recorded by X-ray diffraction (XRD), and the morphologies of ACs were observed by scanning electron microscopy (SEM). The specific surface area and pore size distribution were investigated by N_2/77 K adsorption-desorption isotherms using the Brunauer-Emmett-Teller (BET) equation and non-local density functional theory (NLDFT). Hydrogen uptakes were obtained by an adsorption instrument at 77 K and 60 bar. The results showed that the effective pore sizes for hydrogen storage were expanded at high pressures rather than low pressures.

Poster Presentation : **IND.P-57**
Industrial Chemistry
Zoom 1 WED 17:30~18:00

Ultrafast Rolled-up Production of Graphene Fibers-inserted High-Performance Yarn Type Electrodes

Young-Jung Heo, Soo-Jin Park[*]

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Future wearable technologies including smart or e-textiles integrating two or more of energy storage, sensing, actuating, communicating and computing require careful selection of material and design, manufacturing process, fabrication and scaling up of production process which are economically viable. However these still remain as greatest challenge to the scientific community. Macroscopic reduced graphene oxide fiber (rGOF) has been considered as an attractive candidate for energy storage devices in recent years. However, slow rate of reduction of rGOFs still remains as a hurdle for their large scale production through roll-to-roll process limiting their potential to be used in wearable technologies including smart textiles. Herein, we for the first time report an effective and environment-friendly strategy for combined gel-state ultrafast reduction and one-step roll-to-roll production of graphene fibers. The gel GOFs were completely reduced at room temperature and were used directly as an active electrode material for electrochemical capacitors without any post-treatment, and the bi-scrolling (assembly by wrapping and twisting) of rGOFs with a conductive Korean Traditional Paper (KTP) was successfully employed for designing high volumetric energy density supercapacitors at the scale required for applications. The main advantage of this method is the ease of scalability for industrial applications. The average cell capacitance value of the biscrolled yarn-type supercapacitors which contain 80 rGOFs having cell diameters around 1 mm is ~121,674 mF/cm3 (~122 F/cm3: value normalized by graphene fibers volume only) at a scan rate of 100 mV/s and the capacitance measured at scan rate of 1,000 mV/s is over 75% of that measured at 100 mV/s.

Poster Presentation : **INOR.P-58**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Hybridizing of metal organic framework in clay nanotube for enhanced gas adsorption capacity

Sooji Park

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Metal organic frameworks (MOFs) are hybrid materials that consist of organic ligands and metal ions or clusters. Recently, MOFs have been found to show great potential in CO2 capture due to their high surface area. In this work, we synthesized HKUST-1 in the lumen of Halloysite clay nanotubes (HNTs). HNTs were worked as nanocarriers and the inner surface of HNTs was modified with acid to extend the space volume. HKUST-1 consisted of copper nodes and organic ligands is one of the most widely studied MOFs owing to its high porosity. By confining space inside the nanotube, we could make specific boundary for growing MOFs with longitudinal aixs of HNTs and enhance water stabililty of MOFs. Experimentally, even loading of a MOF precursor among HNTs in a solution phase, and following solvothermal reaction while the precursor is suspended selectively inside of the HNTs. XRD for structural analysis of this hybrid was done showing characteristic reflections. TEM and EDS illustrated the formation and the elemental compositions of this materials. Gas adsorption capacity was analyzed by Brunauer-Emmett-Teller (BET) using N2 and CO2 gases. N2 gas adsorption capacity increased around 4 times, from 95.449 cm3(STP)g-1 to 386.06 cm3(STP)g-1 by acid etching and this hybrid synthesis. This work can be a significant point to synthesize a variety of hybrid nanotube materials to yield synergistic effects and can be applied to competitive adsorbents for gas capturing.

Poster Presentation : **INOR.P-59**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Crystal Structure, Molecular Spectroscopy and Ligand Field Analysis of *trans*-$[Cr(Me_2tn)_2Br_2]_2ZnBr_4$

Jong-Ha Choi, Keon Sang Ryoo*, Chang-Seop Lee[1]

Department of Applied Chemistry, Andong National University, Korea
[1] *Department of Chemistry, Keimyung University, Korea*

The crystal structure of *trans*-$[Cr(Me_2tn)_2Br_2]_2ZnBr_4$($Me_2tn$ = 2,2-dimethylpropane-1,3-diamine) has been determined by a single-crystal X-ray diffraction study at 220 K. The analysis reveals that there are three crystallographically independent Cr(III) complex cations in the title complex. The Cr(III) atoms are coordinated by four N atoms of Me_2tn and two Br atoms in trans arrangement, displaying a distorted octahedral geometry. The orientations of two six-membered chelate rings in three complex cations are in anti chair-chair conformation with respect to each other. The Cr–N and Cr–Br bond lengths average 2.085(4) and 2.464(6) Å, respectively. The $ZnBr_4^{2-}$ have slightly distorted tetrahedral geometry with Zn–Br lengths and the Br–Zn-Br angles influenced by hydrogen bonding. The resolved absorption maxima in the electronic d-d spectrum were fitted with a secular determinant for a quartet energy state of the d^3 configuration in a tetragonal field. It is confirmed that the nitrogen atoms of the Me2tn ligand are strong σ-donors, but the bromo ligands have weak σ- and π-donor properties toward the chromium(III) ion.

Poster Presentation : **INOR.P-60**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Molecular Structure, Spectroscopic Properties and Ligand Field Analysis of *cis*-$[Cr(NCS)_2(cyclam)]_2Cr_2O_7$

Jong-Ha Choi, Keon Sang Ryoo*, Chang-Seop Lee[1]

Department of Applied Chemistry, Andong National University, Korea
[1]Department of Chemistry, Keimyung University, Korea

The structure of *cis*-$[Cr(NCS)_2(cyclam)]_2Cr_2O_7]\cdot H_2O$ (cyclam = 1,4,8,11-tetraazacyclotetradecane, $C_{10}H_{24}N_4$, has been determined from synchrotron data. The asymmetric unit contains one independent $[Cr(NCS)_2(cyclam]^+$ cation, and two halves of a $Cr_2O_7^-$ anion and one water molecule. The Cr(III) ion is coordinated by the four N atoms of cyclam, and two N-coordinated NCS^- ions in a *cis* arrangement, displaying a distorted octahedral geometry. The Cr–N(cyclam) bond lengths are in the range of 2.080 (2) to 2.097 (2) Å while the average Cr–N(NCS) bond length is 1.985 (2) Å. The macrocyclic cyclam moiety adopts the c*cis*-V conformation. The pure electronic energies due to spin-allowed and spin-forbidden transitions are assigned by analyzing the absorption and excitation spectroscopy. Using the observed transition energies, a ligand field calculation was performed to determine the bonding properties of coordinated ligands in the chromium(III) complex.

Poster Presentation : **INOR.P-61**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Preparation of Porous Carbon-Based Composite Incorporated with Cu and Co Nanoparticles

Heewoong Shin, Sojin Oh, Hyeji Jun, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

In general, the activity of nanocatalysts reduces owing to the agglomeration of unstable nanocatalysts during the catalytic reaction. Therefore, the incorporation of nanocatalysts within porous materials to prevent the agglomeration of unstable nanocatalysts is very essential to preserve their original catalytic activity. Herein, we present a convenient method for the incorporation of Cu and Co nanocatalysts within porous carbon material. The pyrolysis of ZIF-67 containing Cu^{2+} ions within the well-developed micropores of ZIF-67 results in a porous carbon composite incorporated with catalytically active Cu and Co nanoparticles.

Poster Presentation : **INOR.P-62**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Size-Controlled Construction of Porous UiO-66 and UiO-67 using Modulators

In-Seop Jang, Sujeong Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

Porous metal-organic frameworks (MOFs) have received a great deal of attention due to their many useful applications in gas storage, catalysis, sensing, and separation. In general, structural features and compositions of MOFs are important factors that define their properties. Furthermore, the size of MOFs is another factor that determine a range of application of MOFs. Herein, we report the preparation of UiO-66 and UiO-67 octahedrons with a controlled size. Relatively uniform nano- and micro-sized octahedrons of UiO-66 and UiO-67 are prepared by using acetic acid as modulators during the particle formation process.

Poster Presentation : **INOR.P-63**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Construction of Hybrid MOFs of Fe,Cr-MIL-101 and Cr-MIL-101@Fe-MIL-101

Junha Song, Moonhyun Oh[*]

Department of Chemistry, Yonsei University, Korea

The construction of hybrid metal-organic frameworks (MOFs), which have more than two different materials and/or structures, is of great interest due to their unique and useful properties. Hybrid MOFs are considered valuable materials, because a weakness of materials can be overcome by making them in hybrid. The mixing of more than two different metal ions during the construction of MOFs can result in hybrid MOFs. In addition, a MOF-on-MOF growth is another approach to make well-defined hybrid MOFs. Herein, we report the construction of core-shell type hybrid MOFs of Cr-MIL-101@Fe-MIL-101 through the MOF-on-MOF growth and Fe,Cr-MIL-101.

Poster Presentation : **INOR.P-64**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Synthesis and Structural Characterization of Zinc(II) and Cadmium(II), Complexes for The Polymerization of rac-Lactide

Hyosun Lee*, **Kyeonghun Kim**

Department of Chemistry, Kyungpook National University, Korea

We have synthesized new series of Zn(II) and Cd(II) complexes, **[(L_{DTEDA})MBr_2]**, supported by ligand N^1,N^1-dimethyl-N^2-(thiophen-2-ylmethylene)ethane-1,2-diamine (L_{DTEDA}). 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 MeLi were investigated at 0°C and 25°C.

Poster Presentation : **INOR.P-65**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Polymerization of *rac*-Lactide by Precatalyst Zinc(II) and Cadmium(II) Complexes

Solhye Choe, Hyosun Lee[*]

Department of Chemistry, Kyungpook National University, Korea

We have synthesized a series of new zinc(II) and cadmium(II) complexes with ligands $\mathbf{L_A}$ and $\mathbf{L_B}$ where L_A = *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-1-(furan-2-yl)-methanamine and L_B = *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl) 1-(furan-2-yl)-methanamine. All synthesized complexes, $\mathbf{[L_nMX_2]}$ (L_n = L_A and L_B; M = Zn, X = Cl; M = Cd, X = Br) were characterized by ^{1}H-NMR, ^{13}C-NMR, IR, and elemental analyzer. In addition, the molecular structures of these complexes were characterized by X-ray single crystal diffraction. The catalytic properties of these complexes toward the polymerization of *rac*-lactide (LA) in the presence of MeLi were investigated at 25°C.

Poster Presentation : **INOR.P-66**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Synthesis and Characterizations of 1,1-Diisopropyl(or Dihexyl)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles

Se yeon Park, Young Tae Park*, Ji Hun Lee

Department of Chemistry, Keimyung University, Korea

The reactions of diisopropyl(or dihexyl)-bis(phenylethynyl)silanes with lithium naphthalenide, $ZnCl_2$, and N-bromosuccinimide (NBS) produced 2,5-dibromo-1,1-diisopropyl(or dihexyl)-3,4-diphenyl-siloles, respectively. In the presence of catalysts such as palladium chloride, copper iodide, and triphenylphosphine, trimethylsilylacetylene (TMSA) was used to replace two bromine groups of the prepared siloles with two trimethylsilylethynyl groups under the solvent of diisopropylamine. The crude products were purified using recrystallization or column chromatography in hexane as solvent. The product materials were characterized by ^{1}H, ^{13}C and ^{29}Si NMR. Photoelectronic properties of the prepared materials were also studied by UV-Vis absorption, excitation and fluorescence emission spectroscopy. In order to study the electrochemical characterizations of the synthesized material, the electrochemical characterizations related to lithium ion batteries were examined.Acknowledgment. This work was supported by the Basic Science Research Program through the Nationaril Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

Poster Presentation : **INOR.P-67**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Synthesis and their Electrochemical Properties of 1,1-Diisopropyl(or 1,1-Dihexyl or 1,1-Diethyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)silole

Ji hun Lee, Young Tae Park*, Se Yeon Park

Department of Chemistry, Keimyung University, Korea

1,1-Diisopropyl(or 1,1-Dihexyl or 1,1-Diethyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)silole were prepared by intramolecular reduction cyclization of diisopropyl(or dihexyl or 1,1-diethyl)bis(phenylethynyl)silane with the treatment of 4.5 mol Li & naphthalene and followed by 4 mol chlorotrimethylsilane in THF as solvent. After the reaction was finished, naphthalene was removed using a sublimation device, and the crude product was purified by recrystallization. The obtained materials are soluble in usual organic solvents such as THF, and $CHCl_3$. The prepared materials were characterized by NMR, and IR spectroscopies. We also studied the electronic properties of the prepared silole derivates by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, as well as electrochemical properties for litthium ion battary in particular.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 : **INOR.P-68**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Concerted Catalysis via Geometrical Matching Interaction of Trinuclear Palladium(II) Catalyst

Dongwon Kim, **Ok-Sang Jung***

Department of Chemistry, Pusan National University, Korea

Reaction of *cis*-protected [(Me$_4$en)Pd(SO$_4$)] with new designed C_3-symmetric barium salt as an anionic ligand (L) produces [(Me$_4$enPd)$_3$L]. This tripalladium(II) complex shows a significant concerted catalytic efficiency on the Heck reaction with appropriate C_3-symmetric trifunctional substrate via the geometrical matching interaction between substrate and catalyst.

Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Supramolecular Isomers of Ag(I) Complexes Based on a Silane Derivative

Heehun Moon, **Seok Kyun Jeong, Ok-Sang Jung**[*]

Department of Chemistry, Pusan National University, Korea

Slow diffusion of AgX ($X^- = NO_3^-$, BF_4^-, ClO_4^-, $CF_3SO_3^-$, and PF_6^-) with 1,3-bis(dimethyl(pyridin-4-yl)silyl)propane at room temperature affords 28-membered metallacyclodimers, $[Ag(L)]_2(X)_2$. For the macrocyclodimer, fine competition among argentophilic, electrostatic, and interaction coexists in the crystalline state. Direction reaction of AgX ($X^- = BF_4^-$ and PF_6^-) with L gives rises to the cyclodimers whereas the anion exchange of $[Ag(L)]_2(NO_3)_2$ with X^- ($X^- = BF_4^-$ and PF_6^-) produces sinusoidal 1D coordination polymers. The macrocyclodimer is a unique molecular chair that tunes a transannular argentophilic interaction via the bite size of the counteranions.

Poster Presentation : **INOR.P-70**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Porous 2D sheets via interlocked 1D ladders: adsorption of xylene isomers by temperature and mixture effects in SCSC mode

Soojin Lee, Junhee Kim, In-Hyeok Park[1], Ok-Sang Jung[*]

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Reaction of silver(I) perchlorate with C_3-symmetric tridentate *N*-donor ligand produces stable crystals with open channels via catenation of 1D ladders. The open-channel crystal significantly shows both temperature and mixture effects on adsorption of *o*-, *m*-, and *p*-xylene isomers in a single-crystal-to-single-crystal (SCSC) mode. *o*-Xylene is not adsorbed into the channel at 5°C, but is inserted into the channel at room temperature. Especially, the 1 : 1 mixture of *o*- and *m*-xylene was adsorbed into the channel in the 1 : 1 mole ratio via intermolecular weak interactions at 5°C.

Poster Presentation : **INOR.P-71**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Syntheses and Properties of Ruthenium Nitrosyl Complexes with Schiff base ligands

Minyeong Kim, Hong In Lee[*]

Department of Chemistry, Kyungpook National University, Korea

Nitric oxide (NO) is an important signaling molecule involved in several physiological processes, including immune response, neurotransmission and inhibition of tumor growth. Various species have been synthesized as nitric oxide donor agents. Among them, metal nitrosyl complexes have been found to be effective in delivering NO by irradiation of light and known as the most effective NO carriers to cell. These findings have proposed metal nitrosyl complexes to be used for photodynamic therapeutic agents in biomedicine. In this study, simplified in situ syntheses of ruthenium nitrosyl complexes [Ru(II)L(NO+)Cl] (L=salophen derivatives) with Schiff base ligands are described. We show the NO-releasing properties of the complexes monitored by IR, UV-VIS, EPR and X-ray crystallography. Also EPR data can be interpreted as that the diamagnetic [Ru-NO]6 electronic state of the complexes change to paramagnetic properties Ru(III) (d5, S=1/2) upon losing NO.

Poster Presentation : **INOR.P-72**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Structural difference depending on the solvent : Heterogenization of supramolecular homogeneous catalyst

Junmyeong Park, Do Heon Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of ZnX_2(X^- = Cl^-, Br^-, I^-, NO_3^-) with ethyl(methyl)(3-pyridine)silane (L) as a bidentate N-donor. It produces new discrete cyclodimeric rings and 2D coordination compound. The coordination network acts as a remarkable transesterification catalytic system that shows both the significant leaving group effect of X^- anions and heterogenization of homogeneous catalysts. The substrate activity is in the order NO_3^- > I^- > Br^- > Cl^-. And a cyclodimeric ring complex that consists of NO_3^- is recrystallized after homogeneous catalytic action.

Poster Presentation : **INOR.P-73**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Nucleophilic reactivity of a mononuclear cobalt(III)–bis(*tert*-butylperoxo) complex

Younwoo Park, **Jaeheung Cho**[1,*]

Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

A mononuclear cobalt(III)–bis(*tert*-butylperoxo) adduct ($\mathrm{Co^{III}}$–$(\mathrm{OO}^{t}\mathrm{Bu})_2$) bearing a tetraazamacrocyclic ligand was synthesized and characterized by various physicochemical methods, such as X-ray, UV-vis, ESI-MS, EPR, and NMR analyses. The crystal structure of $\mathrm{Co^{III}}$–$(\mathrm{OO}^{t}\mathrm{Bu})_2$ complex clearly showed that two $\mathrm{OO}^{t}\mathrm{Bu}$ ligands bound to equatorial position of cobalt(III) center. Kinetic studies and product analyses indicate that the $\mathrm{Co^{III}}$–$(\mathrm{OO}^{t}\mathrm{Bu})_2$ intermediate exhibits nucleophilic oxidative reactivity toward external organic substrates.

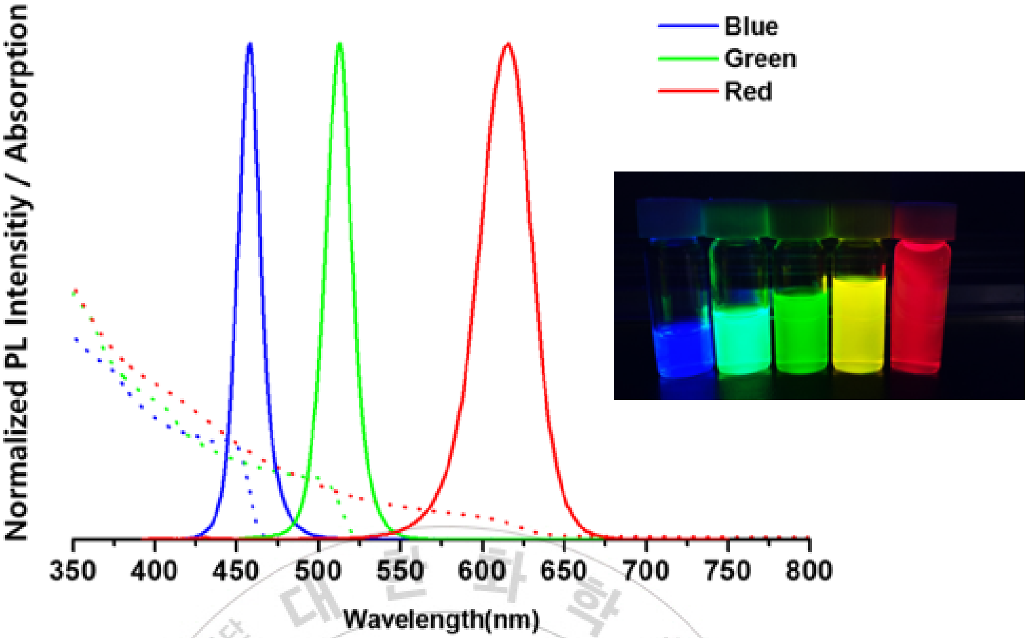
Poster Presentation : **INOR.P-74**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Synthesis of Perovskite Quantum Dots by Z-type ligand and Fabrication of Light-Emitting-Diodes Application

SeungMin Baek, Sangwook Kim[1,*]

Department of Molecular Science and Technology, Ajou University, Korea
[1]*Division of Applied Chemistry & Biological Enginee, Ajou University, Korea*

We synthesized perovskite quantum dots which has high stability at harsh environment using Zinc-trioctylphophine oxide (Zn-TOPO) complex compare to the conventionally used ligand. Zn-TOPO capped PeQDs are showed high quantum yields of over 90% and improved thermal stability than pristine PeQDs. In particular, it is clarified that Zn and TOPO are combined and attached to the surface of the PeQDs through 31P NMR both solution and solid. Additionally, we conducted XPS measurements for more detailed surface analysis of PeQDs, and founded that the Zn-TOPO complex decrease lead-oxide (Pb-O) bonding in the lattice. Finally, we fabricated electroluminescence (EL) devices using these materials and VB-FNPD as a new cross-linkable hole transporting material. The VB-FNPD has a high-hole carrier mobility compared to the PVK as conventional HTL. As a result of EL performance, they have high EQE (%) and current efficiency (Cd/A) of (7.12 %, 9.93 Cd/A) for red, (6.06 %, 32.5 Cd/A) for green, and (0.56 %, 0.88 Cd/A) for blue-emitting devices, respectively.


Normalized PL Intensitiy / Absorption
Blue
Green
Red
350
400
450
500
550
600
650
700
750
800
Wavelength(nm)

Poster Presentation : **INOR.P-75**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Mechanistic insight into hydroxamate transfer reaction mimicking the inhibition of zinc-containing enzymes

Nam Kwon, Jaeheung Cho[1,*]

Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

A hydroxamate transfer reaction between metal complexes has been investigated by a combination of experimental and theoretical studies. A hydroxamate-bound cobalt(II) complex bearing a tetradentate macrocyclic ligand, $[Co^{II}(TBDAP)(CH3C(–NHO)O)]^+$ (**1**), is prepared by the reduction of a hydroximatocobalt(III) complex with a biological reductant. Alternatively, **1** is accessible via a synthetic route for the reaction between the cobalt(II) complex and acetohydroxamic acid in the presence of a base. **1** was isolated and characterized by various physicochemical methods, including UV-vis, IR, ESI-MS, and X-ray crystallography. The hydroxamate transfer reactivity of **1** was examined with a zinc complex, which was followed by UV-vis and ESI-MS. Kinetic and activation parameter data suggest that the hydroxamate transfer reaction occurs via a bimolecular mechanism, which is also supported by DFT calculations. Moreover, **1** is able to inhibit the activity against a zinc enzyme, *i.e.*, matrix metalloproteinase-9. Our overall investigations of the hydroxamate transfer using the synthetic model system provide considerable insight into the final step involved in the inhibition of zinc-containing enzymes.

Poster Presentation : **INOR.P-76**

Inorganic Chemistry

Zoom 2 WED 16:30~17:00

Highly durable covalent-organic framework for the simultaneous ultrasensitive detection and removal of noxious Hg^{2+}

Younghu Son, Yang Yanqin[1], Minyoung Yoon[*], Taehyun Bae[2,*]

Department of Chemistry, Kyungpook National University, Korea
[1]*School of Chemical Engineering and Technology, Hebei University of Technology, China*
[2]*School of Chemical and Biomedical Engineering, Nanyang Technological University, Singapore*

In recent years, aquatic pollution by various heavy metals has posed an increasingly severe threat to biodiversity. Among toxic metal ions, Hg^{2+} represents a severe threat to humankind and other living species because Hg^{2+} can cause serious health problems. Designed porous materials, such as covalent organic frameworks (COFs) and metal-organic frameworks (MOFs), are promising materials for the removal of toxic metals from wastewater. To assess the contamination and removal of toxic metal ions, their ultrasensitive detection is extremely important. To date, there have been very few reports on the ultrasensitive (picomolar) detection of toxic metal ions using highly porous COFs. Therefore, in this study, we synthesized a highly porous and durable COF containing amine and sulfonyl groups using the hydrothermal method. We demonstrated the performance of obtained COF for the selective and ultrasensitive detection of Hg^{2+}. Owing to its excellent luminescence properties and highly π-conjugated system, this metal-free COF can be used as a signal transducer for the selective and sensitive detection of Hg^{2+} at the picomolar level. We studied the influence of various factors (e.g., pH, concentration, and temperature) on the sensitive detection of Hg^{2+}. Owing to excellent luminescence properties and ultrasensitive detection of Hg^{2+}, COF works as highly adsorbent materials for Hg^{2+} with the effective removal capacity of 99.8% at neutral pH. The obtained COF was also applied as a probe for the simultaneous detection and removal of Hg^{2+} in a natural river water sample. The results indicate a new path toward metal-free chemical sensors for toxic pollutants. Details of this work will be presented.

Poster Presentation : **INOR.P-77**
Inorganic Chemistry
Zoom 2 WED 16:30~17:00

Reversible Single-crystal-to-single-crystal (SCSC) Transformation in Aza-macrocyclic Copper(II) Complex

Ahrim Jeong, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

The design and synthesis of macrocyclic compounds have been attracted much attention in chemistry because of their significant structures and potential applications such as sensor, catalysis, magnetism, chirality and gas sorption. Recently, we prepared a new copper(II) aza-macrocyclic complex, $[Cu(C_{16}H_{38}N_4)(H_2O)_2](C_{12}H_6O_4)$ (1), using a copper(II) aza-macrocyclic complex containing butyl pendant groups, $[Cu(C_{16}H_{38}N_4)(ClO_4)_2]$, and 2,7-naphtalenedicarboxylic acid (2,7-NDC). When monomeric compound (1) was immersed in methanol, polymeric compound, $[Cu(C_{16}H_{38}N_4)(C_{12}H_6O_4)]_n{\bullet}(CH_3OH)$ (2), was obtained by single-crystal-to-single-crystal (SCSC) transformation. Furthermore, when polymeric compound (2) was immersed in water, a reversible SCSC transformation from (2) to (1) occurred. The reversible SCSC transformation between (1) and (2) was investigated by single-crystal X-ray diffraction and in situ powder X-ray diffraction. Complex (1) gives a 3D supramolecular structure formed by strong intermolecular hydrogen bonds, whereas complex (2) features a 1D zigzag coordination polymer. Additionally, despite its poor porosity, complex (2) displayed interesting CO_2 adsorption behaviour under CO_2 gas. In this poster, we will present the detailed preparation of the copper(II) aza-macrocyclic compounds, crystal structures, reversible SCSC transformation and gas sorption.

Poster Presentation : **INOR.P-98**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

The doping effect of noble metal in ruthenium oxide nanoparticles for oxygen evolution reaction in acidic media

Chung man Yu, Yongju Hong, Jinhyoung Jo, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Ruthenium-based nanomaterials have great attention in the energy conversion field due to their intrinsically superior catalytic activity toward oxygen evolution reaction (OER). However, despite their promise, the major concern with Ru-based catalysts (RuO_2) is the continuous dissolution during the OER operation. Recent studies have shown that the leaching problem can be alleviated by doping additional metals, which drastically suppressed the over-oxidation of Ru in the ruthenium oxide matrix, thus preserving the beneficial activity of ruthenium oxide. Here in, we have successfully introduced noble metals with controlled amounts toward dendritic ruthenium nanospikes. Moreover, the noble metal-alloyed ruthenium nanospikes further transformed into noble metal-doped ruthenium oxide followed by thermal oxidation process, which showed enhanced OER activity and durability under acidic condition. The significant role of noble metal elements, stabilizing ruthenium oxides, will be presented.

Poster Presentation : **INOR.P-99**
Inorganic Chemistry
Zoom 2 WED 17:00~17:30

PdPb nanosponge-embedded RuO2 as highly active and stable electrocatalyst toward the oxygen evolution reaction

Heesu Yang, Minki Jun, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Hydrogen production through the water-splitting method is carbon-free; hence, it is regarded as a promising pathway to reduce global warming. However, the sluggish kinetics of OER half-reaction is a significant issue and requires highly active and stable catalysts. Regarding this situation, it is well known that Ru-based nanocatalysts exhibit great reactivity, but at the same time, show poor stability in acidic OER. Therefore, to stabilize and efficiently adopt Ru-based nanocatalyst, we deposited RuO_2 on the PdPb nanosponge. PdPb-RuO_2 nanosponges were synthesized through the deposition of Ru shell on the surface of PdPb nanosponge and subsequent thermal oxidation to form RuO_2. Highly porous nanosponge contributed to maximizing Pd-doping on RuO_2 by enlarging the heterointerface area between Pd and RuO_2. As a result, the prepared catalyst exhibited enhanced catalytic activity and stability than other Ru-based catalysts toward OER in acidic media.

Poster Presentation : **INOR.P-100**
Inorganic Chemistry
Zoom 2 WED 17:00~17:30

Pseudo-Epitaxial Growth of CdTe/CdS Nanoplate via Intraparticle Migration of CdTe

Seokpyo Jeon, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Ion exchange reaction is one of the powerful tools for approaching unexplored hetero-structured nanomaterials. To succeed in producing heteronanoparticles with anisotropic morphology, it is required to modulate the surface energies of certain facets in nanoparticles elaborately. However, in case of anion exchange, the sluggish diffusion of anions often requires the harsh reaction condition so that the exquisite control of morphology or composition rarely takes place. Herein, we report an apparent pseudo-epitaxial growth of CdTe on the CdS template via anion exchange reaction. We witnessed that the CdS phase reacts with Te to form CdTe at the lateral sites of CdS first via anion exchange reaction, attaching randomly but selectively at the edge of CdS in terms of surface energy among the facets. Then, these newly-grown CdTe islands gradually migrate onto the flat plane of (002)CdS, forming two dimensional single crystalline CdTe nanoplates, which seems to be constructed by the direct epitaxial growth. From the detailed intermediate analysis with HRTEM and atomic modeling, we revealed the reason for this intriguing intraparticle migration of CdTe islands onto CdS relates to the tolerable lattice mismatch between anion frameworks, asymmetric environment of exposed atoms in CdS(002), and overall surface energy minimization of CdS/CdTe. We expect that our work will provide a fresh viewpoint to the epitaxial growth so that the mechanistic pathways of heteroepitaxy might have to be revised completely for certain chemical compound systems.

Poster Presentation : **INOR.P-101**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Rh-doped IrOx to enhance the activity in acidic oxygen evolution reaction via mild annealing

Jinhyoung Jo, Taekyung Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Currently, Ir-based catalysts have been spotlighted as a promising candidate among the anodic materials for the commercial water electrolyzer due to their higher stability than Ru-based catalysts toward the oxygen evolution reaction (OER), however, increasing their activity still remains challenging to date. Doping foreign elements into the Ir oxides is an attractive strategy that can optimize the binding energy of the OOH(ads) which is known as rate determining step (RDS) intermediates for the OER. In this work, we show the synthetic strategy for modulating the electronic structure of IrOx to enhance the catalytic activity via thermal annealing, which might induce the mixing with the components of metal sulfide supports, thereby boosting the sluggish kinetics of OER and alleviating the degradation of Ir-based electrocatalysts in acidic electrolyte. We prepare the Rh-doped IrOx-based nanocages from the blending Ir clusters with the Rh-PbS nanocubes through the pyrolysis in the air and sequential etching with acid. These Rh-doped IrOx-based nanocages exhibit a great activity and stability towards the acidic OER, which quite surpasses the performances of currently reported Ir-based OER catalysts. From this work, we expect that the appropriate pyrolysis condition can control dopant in the IrOx, and thus allow to optimize activity and stability toward the acidic OER.

Poster Presentation : **INOR.P-102**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Correlation between the Matrix Metalloproteinases and Biomolecules in Alzheimer's Disease

Eungchan Kim, Dong Woo Son, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) are proposed as many pathological indicators for the diseases including Alzheimer's disease (AD), intervertebral disc degeneration, and restenosis. Among MMP family, MMP-2 and MMP-9 have been revealed to be associated with AD because of high levels in the brain tissue of AD patients. In addition, MMPs degrade both amyloid precursor protein (APP) and amyloid-β (Aβ) which could lead AD. One of the well-known symptoms of AD is cognitive impairment. In this study, we will examine the influence of various biomolecules on MMPs' degrading ability of Aβ as well as propose the mechanisms how those natural products affect the activity of MMPs using biochemical and biophysical methods (i.e., zymography, Western blot, and mass spectrometry) under various conditions (e.g., stoichiometry) in order to understand the relationships between the natural products and MMPs. Our overall investigation from the experiments could provide better insight into the study of the metalloenzymes related to AD pathology.

Poster Presentation : **INOR.P-103**

Inorganic Chemistry

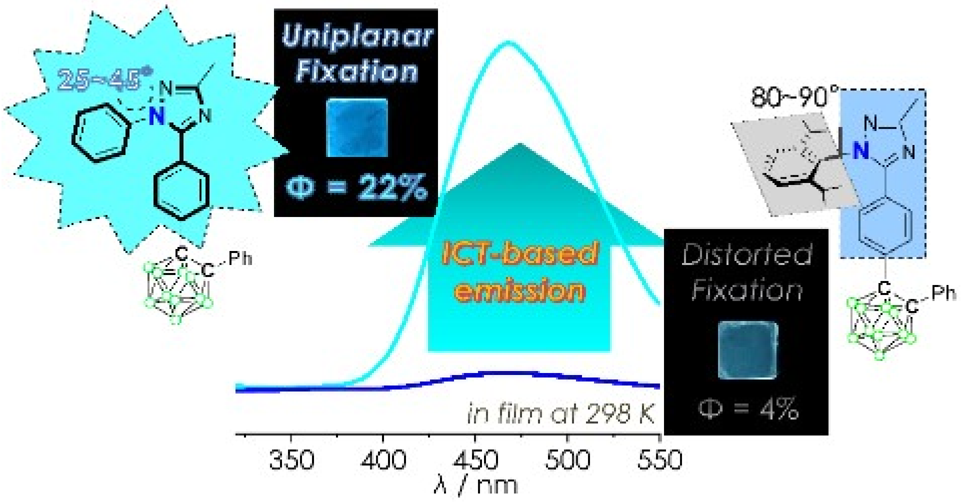
Zoom 2 WED 17:00~17:30

The Planarity Difference of 1,2,4-Triazole-based *o*-Carboranyl Luminophores: Basis to Control Intramolecular Charge Transfer

Mingi Kim, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Strategically designed two *o*-carboranyl compounds containing 1,2,4-triazole groups, each appended with an *N*-aryl ring (either *N*-phenyl or *N*-diisopropylphenyl), were prepared and fully characterized to explain the relationship between their structural orientation (planarity) and intramolecular charge transfer (ICT)-based radiative decay. The photophysical analysis of both compounds shows that the *N*-phenyl appended compound possesses a much higher quantum yield and larger radiative decay constant for ICT-based emission in the rigid state (solution at 77 K and film) than those of the *N*-diisopropylphenyl appended compound, even exhibiting an additional ICT-based emission in solution at 298 K. Theoretical calculations indicate that increasing the coplanarity of the appended aryl-triazole moiety enhances the efficiency of the ICT transition, thus improving the quantum yield and radiative decay efficiency. These findings obviously demonstrate that the planarity of the aryl groups appended to the triazole moiety of an *o*-carboranyl Donor-Acceptor system is a critical factor for controlling the ICT-based radiative decay of these luminophores.



Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Dipyrromethene Chelating-based Triarylboryl-Iridium(III) Complexes and their ‘Turn-on’ Phosphorescent Features via Fluoride Binding

Ju Hyun Hong, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Two novel heteroleptic cyclometalated iridium(III) complexes, namely (C^N)$_2$Ir(**BL**) (**Ir1** and **Ir2**) (C^N = 2-(2,4- difluorophenyl)pyridine (dfphpy, for **Ir1**) and 2-phenylpyridine (phpy, for **Ir2**)), chelated by the triarylboryl dipyrromethene ancillary ligand (**BL**) were synthesized and characterized. Their UV–vis absorption spectra exhibited typical metal-to-ligand charge transfer (^{1}MLCT) absorption bands at 483 nm in addition to borane-centered charge transfer (CT) absorption bands at ~326 nm. The photoluminescence (PL) spectra for these complexes demonstrated phosphorescent emission in the near infrared region (λ_{em} = ~690 nm), which was attributed to the ^{3}MLCT transition. In addition, fluoride titration experiments using these complexes exhibited gradually quenched absorption bands in the region of 300–350 nm, corresponding to borane centered CT transitions. Upon the addition of fluoride, the PL spectra showed a ratiometrically ‘turn-on’ emissive response and gradual blue-shifted patterns. Computational calculations and cyclic voltammetry measurements using the neutral Ir(III)-conjugates and their fluoride adducts strongly suggested that the intriguing emissive response is the result of fluoride binding interrupting the original ^{3}MLCT transition, reinforcing the dipyrromethene-centered π–π* transition, and further inducing the enhancement of the band-gap. Consequently, intramolecular electronic transitions on the Ir(III)-borane conjugated complexes could be fine-tuned via fluoride anion binding, suggesting that the described complexes are good candidates for iridium-based phosphorescent sensory materials to detect fluoride anions through ‘turn-on’ emission in the near IR region.

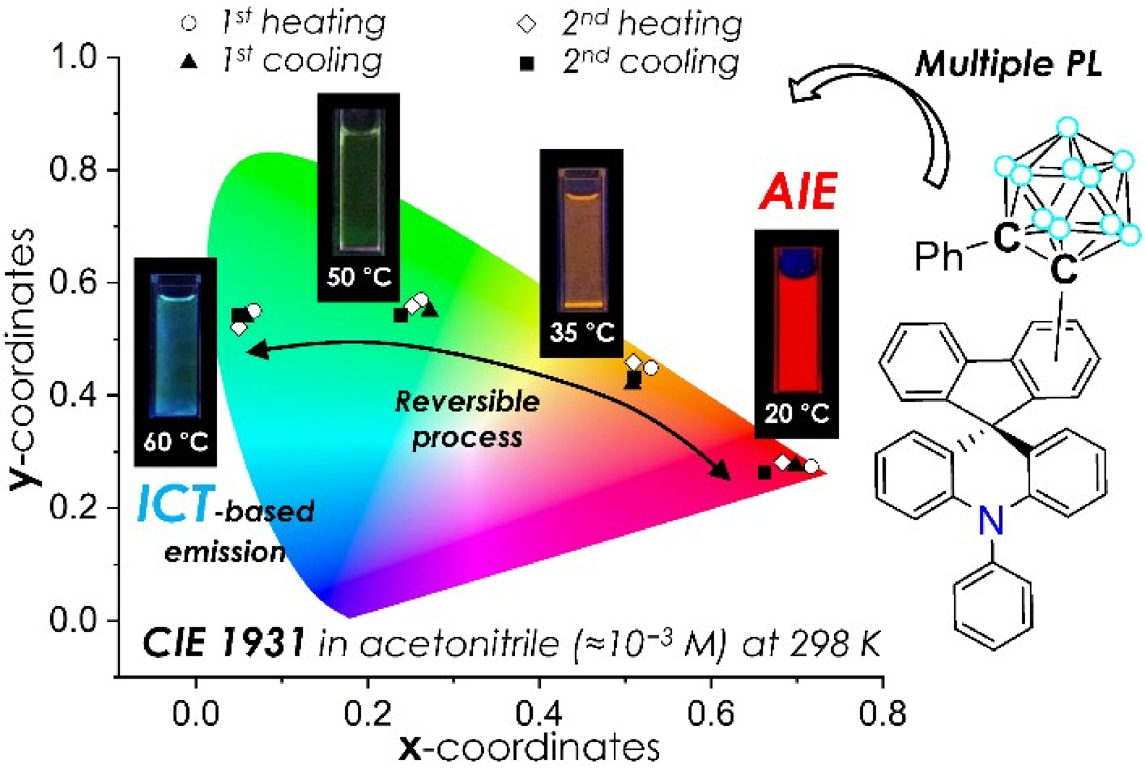
Poster Presentation : **INOR.P-105**
Inorganic Chemistry
Zoom 2 WED 17:00~17:30

Photophysical Properties of Spiro[acridine-fluorene]-based *o*-Carboranyl Compounds and Potential as a Color-Tunable Sensor

Min Sik Mun, Kang Mun Lee[*]

Department of Chemistry, Kangwon National University, Korea

This group synthesized two spiro[acridine-9,9'-fluorene]-based *closo*-*o*-carboranyl compounds, namely *p*-**SAC** and *o*-**SAC**. In addition, these complexes were fully characterized by multinuclear nuclear magnetic resonance (NMR) spectroscopy and elemental analysis (EA). Further, the solid-state structure of *o*-**SAC** was determined using single-crystal X-ray diffraction. *p*-**SAC** exhibited a weak high energy emission trace (λ_{em} = *ca*. 390 nm) only in tetrahydrofuran (THF) at 298 K, while the photoluminescence (PL) spectra at 77 K exhibited intense emission in the low energy region (λ_{em} = 430–500 nm). However, *o*-**SAC** exhibited an excellent dual-emissive pattern in THF at both 298 and 77 K. The PL spectra of both *o*-carboranyl compounds in the film state exhibited broad emissive patterns around 500 nm. The PL experiments in the THF/water mixtures indicated that these features were caused by the aggregation-induced emission (AIE) effect. The ICT-based emissive feature of *o*-**SAC** in solution at 298 K was also subjected to a significant degree of the solvatochromism effect in various organic solvents. An acetonitrile solution containing relatively high concentrations of *o*-**SAC** (*ca*. 10^{-3} M) exhibited a dramatic emission color change from deep red to sky blue when the temperature was increased. The higher temperature caused a natural conversion from a colloidal state (slightly aggregated) to a clear solution. Consequently, the photophysical features of *p*-**SAC** and *o*-**SAC** demonstrated the application potential of π–aromatic conjugated *o*-carboranyl compounds as visual sensory materials.



○ 1st heating
▲ 1st cooling
◇ 2nd heating
■ 2nd cooling
Multiple PL
1.0
0.8
0.6
0.4
0.2
0.0
y-coordinates
50 °C
35 °C
AIE
20 °C
60 °C
Reversible process
ICT-based emission
Ph
C
C
N
CIE 1931 in acetonitrile (≈10−3 M) at 298 K
0.0
0.2
0.4
0.6
0.8
x-coordinates

Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Synthesis of Monodentate Benzo[*d*]imidazole-based Iridium Complexes and Their Dual Emission Property

Chan Hee Ryu, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Herein, we prepared three heteroleptic iridium complexes possessing a monodentate benzo[*d*]imidazole ligand: **IrBzH** (bis[2-(4,6-difluorophenyl)pyridinato-C^N](1-pyridin-2-yl)-1H-benzo[*d*]imidazolate)iridium(III)), **IrBzCN** (bis[2-(4,6-difluorophenyl)pyridinato-C^N](2-(1H-benzo[*d*]imidazolate-1-yl)isonicotinonitrile)iridium(III)), and **IrBzBr** (bis[2-(4,6-difluorophenyl)pyridinato-C^N](1-(4-bromopyridin-2-yl)-1H-benzo[*d*]imidazolate)iridium(III)). The complexes were fully characterized by multinuclear NMR spectroscopy and elemental analysis. The molecular structures were definitively determined by single-crystal X-ray diffraction. The photoluminescence spectra of all three complexes in toluene at ambient temperature exhibited a dual emissive pattern in the high- and low-energy regions. For **IrBzCN** and **IrBzBr**, the emissions were simultaneous in accordance with the excitation energies (λ_{em} = 342 nm and 370 nm), indicating that exhibiting both fluorescent (in the high-energy region) and phosphorescent (in the low-energy region) emissions is an inherent property of these complexes. Time-dependent density functional theory calculations verified that each fluorescent emission of the Ir complexes is associated with a ligand-to-ligand charge transfer transition, and the phosphorescent emission can be assigned to typical triplet metal-to-ligand charge transfer transitions between Ir^{3+} and the difluorophenylpyridine ligand.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

The other usage of vermicide as a regulator of neprilysin related to Alzheimer’s disease and heart failure.

Choi Jae Yoon, Hang Choi, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Neprilysin (NEP) is a zinc metalloproteinase that has been suggested to be involved in several diseases such as Alzheimer’s disease (AD), and heart failure (HF). NEP could degrade amyloid-β (Aβ) which could be related to the pathology of AD. Moreover, NEP is considered to lead natriuretic peptides become inactive and consequently, the occurrence of HF. Thus, the regulation of NEP could be an important point to improve the understanding of AD pathology and curing HF. From previous studies, most of NEP regulators have common structure, phenyl residue, such as polyphenols (e.g., caffeine). Recently, well known vermicides, Albendazole and Mebendazole, have been suggested to be potent anti-cancer drugs. In addition, they have structural similarity to NEP regulators indicating that they could have possibility to control the activity of NEP. Therefore, in this study, we will determine whether both Albendazole and Mebendazole could act as NEP regulators by biophysical and biochemical experiments mass spectrometry, ELISA, enzyme activity assays, and Western blot.

Poster Presentation : **INOR.P-108**

Inorganic Chemistry

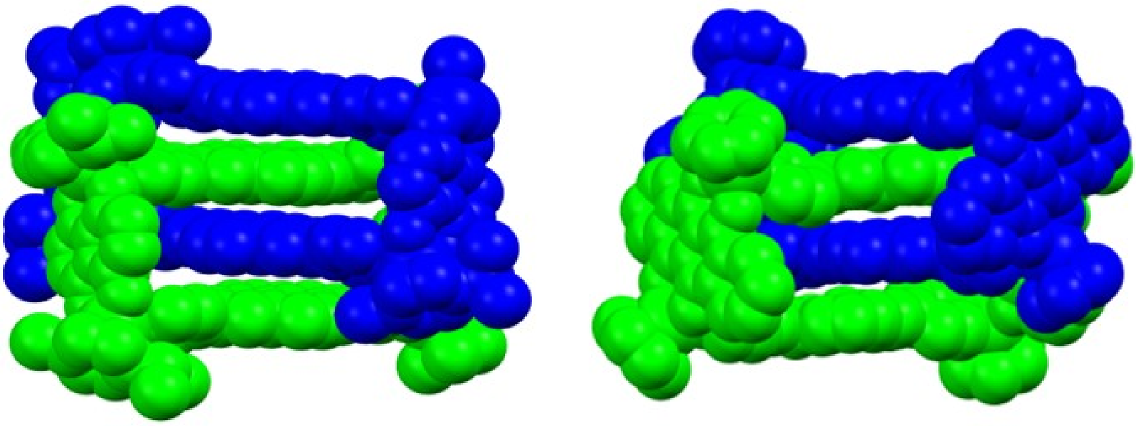
Zoom 2 WED 17:00~17:30

Pyrene-based linear [2] Catenated Metalla-Rectangles with Arene Ruthenium Corners

Gajendra Gupta, Miyeon Kim, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

In recent years, metal based self-assembled threaded architectures such as Borromean rings, Catenanes, Solomon links and other interlocked systems have gained much attraction due to their interesting molecular structures leading to several important applications as described by the molecular machines developed by Nobel Laureates Sauvage, Stoddart and Feringa.[1] Arene ruthenium and Cp* iridium and rhodium precursors were also readily used by Chi and Jin to develop such interesting systems.[2,3] Herein, we describe the synthesis of two new linear dipyridyl pyrene-based catenated metalla-rectangles with arene ruthenium corners. The single crystal XRD structures confirm the formation of the catenated system where two rectangles are threaded to each other . These catenated architectures were found to be stable in methanol even after 30 days. However, in nitromethane the catenated structure slowly transforms into mono rectangle with over 80% conversion after 48 h. The photophysical properties of the system were also being studied.**References:**1.Sauvage, J.-P.; Stoddart, J. F.; Feringa, B. L. *The Nobel Prize in Chemistry* **2016**.2.Gao, W.-X.; Feng, H.-J.; Guo, B.-B.; Lu, Ye.; Jin, G.-X. *Chem. Rev.* **2020**, 120, 6288-6325.3.Gil-Ramirez, G.; Leigh, D. A.; Stephens, A. J. *Angew. Chem. Int. Ed.* **2015**, 54, 6110-6150.



Poster Presentation : **INOR.P-109**

Inorganic Chemistry

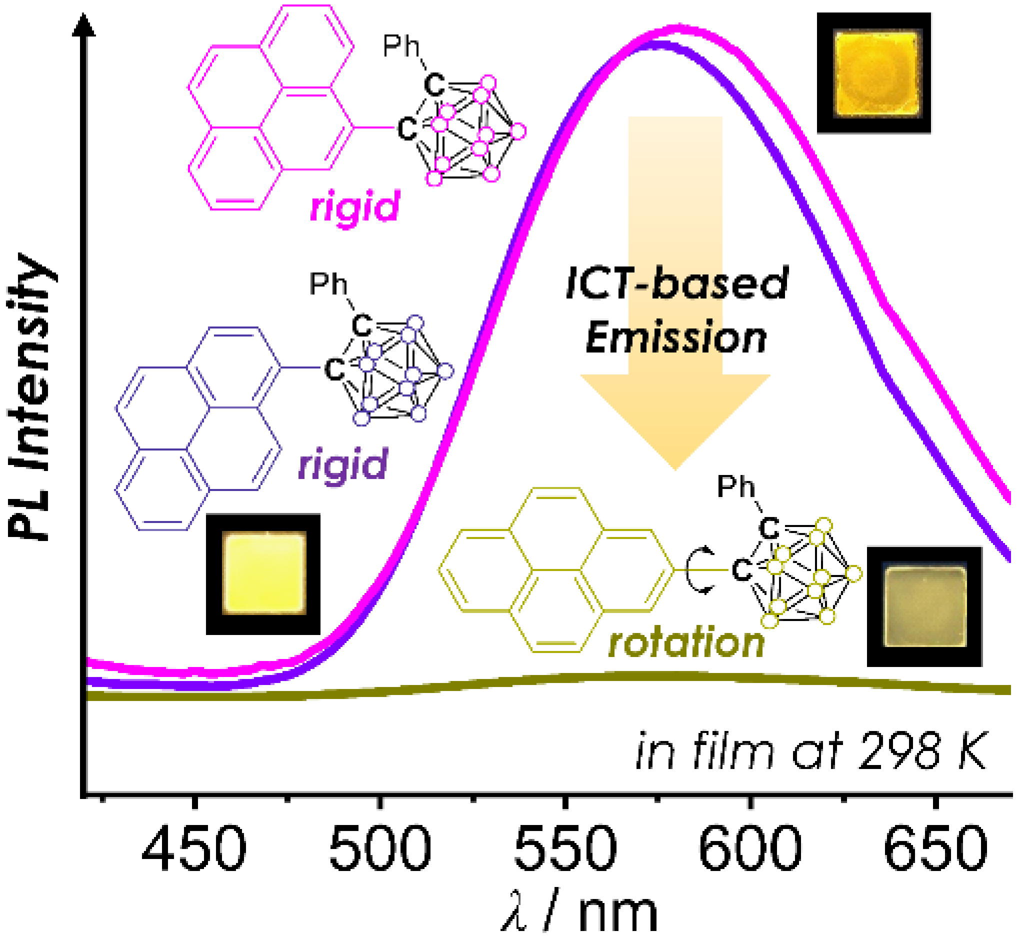
Zoom 2 WED 17:00~17:30

closo-o-Carborane-Funtionalised Pyrenes and their Substituted Position Effect for Photophysical Properties

Hyunhee So, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Three *closo-o*-carborane-substituted pyrene compounds (**1CB**, **2CB**, and **4CB**) were synthesized and fully characterized. The solid-state structures of these compounds were determined by single-crystal X-ray diffraction, and showed a perpendicular structure between the C-C bond of the *o*-carborane and the pyrene ring. This agreed with the theoretical optimized structures of the S_0- and S_1-states. **2CB** showed less intense LE-based emissions in THF at 298 K, while **1CB** and **4CB** displayed strong ICT-based emission involving the *o*-carborane moiety. Although the PL spectra of all compounds demonstrated enhanced ICT-based emission via inhibition of C-C bond variance within the *o*-carborane in rigid states (THF at 77 K and films), the quantum efficiency of **2CB** in films (Φ_{em} = 5%) did not significantly increase compared to that in THF at 298 K, while the values for **1CB** and **4CB** in films were dramatically enhanced to 75% and 62%, respectively. The relative energy barriers to rotation of the dihedral angles between the *o*-carborane cages and pyrene rings indicated that the *o*-carborane cage in **2CB** could rotate more easily than those in **1CB** and **4CB**. Furthermore, the involvement of the *o*-carborane moiety in the LUMO level of **2CB** was significantly affected by this dihedral angle. These results suggest that the free rotation of the *o*-carborane cage of **2CB** interrupted its ICT transitions.


PL Intensity
Ph
C
C
rigid
Ph
C
C
rigid
ICT-based
Emission
Ph
C
rotation
in film at 298 K
450
500
550
600
650
λ / nm

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

New Copper Methyl Thiolate Halides by DMSO Solvothermal Reactions

Jiehye Shin, Junghwan Do[1,*]

Chemistry, Konkuk University, Korea

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

During the exploratory solvothermal synthesis studies, we discovered interesting copper coordination polymers, $Cu_{12}Cl_6(SCH_3)_6(DMSO)$ (**1**), $Cu_3Br(SCH_3)_2$ (**2**), $CuBr(SCH_3)$ (**3**), $Cu_3I(SCH_3)_2$ (**4**), $CuI(SCH_3)$ (**5**). The methyl thiolate (SCH_3) ligand was formed under solvothermal reaction condition by decomposition of dimethyl sulfoxide (DMSO) solvent. Herein, we report five copper methyl thiolate halide compounds, which are characterized by single crystal X-ray diffraction(SXRD), thermogravimetric(TG) analysis, IR, UV-vis, and (TR)PL spectroscopy. Although the evidence is qualitative, we found strong scintillation phenomenon (white radiation for **1**) during the X-ray diffraction measurements in Pohang accelerator laboratory. There are three different types of structures, $Cu_{12}Cl_6(SCH_3)_6(DMSO)$ (**1**), $Cu_3X(SCH_3)_2$ (X=Br, I) (**2, 4**), $CuX(SCH_3)$ (X=Br, I) (**3, 5**), which show 2D and 3D structures. Notably, depending on the structure (irrelevant to halide species) the emission range and lifetime was significantly different to each other.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Interfacial strain induced by the lattice distortion in the Cu1.81S/CuCrS2 hetero-nanostructure

Ye Ji Park, Taehyun Kwon[1], Kwangyeol Lee[1,*]

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

Nanostructures with heterointerfaces have received a great attention because the lattice strain between different phases is one of the important factors that define the catalytic performance of nanocatalysts by affecting the surface energy. In this study, we synthesized the edge-grown Cu1.81S/CuCrS2 nanoparticle and edge-surrounded Cu1.81S/CuCrS2 nanoparticle via elaborate kinetic control of cation exchange reaction of copper sulfide with Cr cations. The lattice mismatch in the heterointerface between Cu1.81S phase and CuCrS2 phase induces the interfacial strain by distorting the sulfur anion framework. The degree of the interfacial strain can be modulated by additional copper sulfide phase overgrowth or etching reaction that removes the copper sulfide phase. The fine control of the interfacial strain between between Cu1.81S phase and CuCrS2 phase is discussed in detail.

Poster Presentation : **INOR.P-112**
Inorganic Chemistry
Zoom 2 WED 17:00~17:30

Supramolecular Nanostructure of Pt(II)-Terpyridine-Based Complex

Seok gyu Kang, Jong Hwa Jung[1,*]

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

The terpyridine-base ligand **1** possessing unsaturated alkyl chain group was prepared by five steps. The Pt(II) complex was also prepared using $PtCl_2$ in DMSO/H_2O solvent. We measured PL, CD, and UV-vis spectra of Pt(II) complex in mixed DMSO/H_2O. Pt(II) complex showed intense PL spectrum and CD signal, which was attributed to the directional Pt-Pt interaction we will present spectroscopic properties of Pt(II) complex.

Poster Presentation : **INOR.P-113**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Ir/Ru-based nanoparticles grown on metal sulfides as efficient electrocatalysts for oxygen evolution reaction

YunChang Son, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Water electrolysis is regarded as one of the most promising energy conversion methods for the hydrogen society. However, the bottleneck in improving water electrolysis is the sluggish kinetics of the oxygen evolution reaction (OER). Although IrOx and RuOx have proven to be the most active electrocatalysts to overcome this limitation, they can be easily dissolved during the OER in acidic conditions, leading to the deterioration of electrocatalytic performance. Therefore, we synthesized Ir/Ru based nanoparticles on mixed metal sulfide as a template for optimizing the electronic structures and oxidation states of Ir and Ru to enhance the catalytic activity and stability. Herein, we report the synthesis of Ir/Ru nanoparticles grown on the Pd13Cu3S7 nanoplates and their potential as the electrocatalysts toward the OER.

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Degradation of PET into terephthalic acid catalyzed by the solid acid

Hyejin Yu, Hyun Sung Kim*

Department of Chemistry, Pukyong National University, Korea

PET degradation is one of the efficient method to solve environmental threat caused by plastic wastes. PET is depolymerized into terephthalic acid (TPA) and ethylene glycol (EG) by hydrolysis reaction, which can be accelerated by designed proper catalyst. A variety of solid acids was employed as catalyst and their efficiencies were investigated in microwave assisted hydrothermal reaction. We offer new approach to handle post-consumer recycled PET waste.

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Porous 2D Organic Templates via Cocrystallization of Melamine with Disulfonic Acids: Adsorption of Diverse Alcohols in SCSC Mode

KangSan Hong, In-Hyeok Park[1], Ok-Sang Jung[2,*]

화학과/초분자재료, Pusan National University, Korea
[1]*Graduate School of Analytical Science and Technology, Chungnam National University, Korea*
[2]*Department of Chemistry, Pusan National University, Korea*

Cocrystallization of melamine with organic sulfonic acids (1,5-naphthalenedisulfonic acid and 4,4'-biphenyldisulfonic acid) gives rise to 2D porous organic frameworks. Each 2D framework has a different channel-size according to the length of the organic sulfonic acids. The adsorption of various liquid alcohols (1-butanol, 1-hexanol, 1-octanol, 1-decanol, 1-dodecanol, tert-butanol, and 2-ethyl-1-hexanol) into the channels in the single-crystal-to-single-crystal (SCSC) mode was effective for each channel. The tailor-made metal-free organic pores presented herein can be useful components of a practical template for 3D structure determination of various liquid alcohols.

Poster Presentation : **INOR.P-116**
Inorganic Chemistry
Zoom 2 WED 17:00~17:30

Effect of Transition Metal for Determining Crytal Structure and Electronic Properties on the Zintl phase $BaZn_{1-x}Cd_xSb_2$ System.

Seongbeom Yeon, Tae-Soo You[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

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. These kinds of Zintl phases are known to be suitable for high-temperature thermoelectric applications. 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. 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 this transition metals for the refined structure types, the solid-solution quaternary Zintle phase $BaZn_{2-x}Cd_xSb_2$ system containing the Zn/Cd mixed-site was synthesized by conventional high-temperature synthetic method, and their crystal structures were characterized by both powder and single-crystal X-ray diffractions. Interestingly, $BaZn_{0.65(3)}Cd_{1.35}Sb_2$ initially adopted the orthorhombic $BaCu_2S_2$-type phase (space group $Pnma$, $Z = 4$, Pearson Code $oP36$). However, after the post-heat treatment, this title compound was transformed into the trigonal $CaAl_2Si_2$-type phase (space group $P\text{-}3m1$, $Z = 1$, Pearson Code $hP5$). A series of theoretical calculations using three hypothetical models was performed by the tight-binding linear muffin-tin orbital (TB-LMTO) method, and the resultant DOS and COHP curve analyses were thoroughly studied.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Zoom 2 WED 17:00~17:30

Ammonia uptake of a metal organic framework adsorbent from ultralow to ambient pressure

Daewon Kim, Yun Seok Chae[1], Doo San Choi[2], Chang Seop Hong[1,*]

Department of chemistry, Korea University, Korea
[1]*Department of Chemistry, Korea University, Korea*
[2]*Korea University, Korea*

Although numerous porous adsorbents have been investigated for NH_3 capture applications, these materials often exhibit insufficient NH_3 uptake, low NH_3 affinity at the ppm level, and poor chemical stability against wet NH_3 conditions. Herein, we report the NH_3 capture properties of iso-reticular series of a tetra-dentate carboxylate-based MOFs that contain open metal sites. The NH_3 uptake of one of the MOFs examined are record high capacities at both pressures among existing porous adsorbents. The properties related to ammonia capture application such as stability, strength of interaction, selective ammonia capture in wet conditions were characterized with PXRD, FT-IR, sorption, breakthrough, and TPD curves. Detailed synthesis and properties will be presented in poster.

Poster Presentation : **INOR.P-138**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

[Withdrawal] Development of ZIF-encapsulated gold nanorod assembly for molecular selective sensing

Suhyeon Park, Juyeong Kim*

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Korea

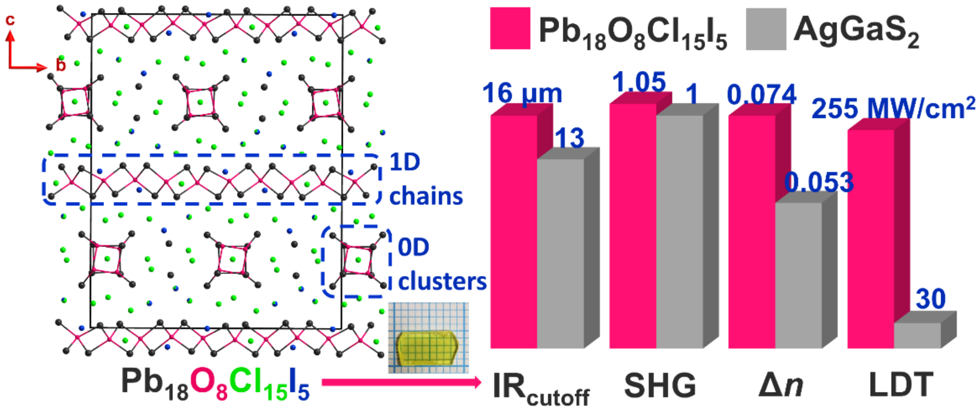
Poster Presentation : **INOR.P-139**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

A Polar Lead Mixed Oxyhalide with Unprecedented Architecture and Excellent Overall Nonlinear Optical Properties

Xinglong Chen, Qun Jing[1,*], Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea
[1]*College of Physical Science and Technology, Xinjiang University, China*

Aiming at developing high-performance nonlinear optical (NLO) materials applied in infrared (IR) region, we have implemented a rational element-composition design strategy and investigated the unexplored PbO–$PbCl_2$–PbI_2 system. By doing so, a new polar lead mixed oxyhalide, $Pb_{18}O_8Cl_{15}I_5$, representing the first artificial metal oxyhalide with combination of Cl^- and I^-, was obtained by an experience-based solid-state synthetic method. Centimeter-sized single crystals of $Pb_{18}O_8Cl_{15}I_5$ have been successfully grown via the top-seeded solution growth (TSSG) technique in air condition. The crystal structure of $Pb_{18}O_8Cl_{15}I_5$ unprecedentedly features two different dimensional types of oxocentered Pb–O units, namely, 1D $[OPb_2]^{2+}$ chains and 0D $[O_4Pb_8]^{8+}$ clusters. Remarkably, characterizations based on the large-sized single crystal reveal that $Pb_{18}O_8Cl_{15}I_5$ outperforms the commercial IR NLO material $AgGaS_2$ in the overall key properties including IR transparent range, second-harmonic generation (SHG) response, birefringence, and laser-induced damage threshold (LDT).


c
b
1D
chains
0D
clusters
$Pb_{18}O_8Cl_{15}I_5$
$Pb_{18}O_8Cl_{15}I_5$
$AgGaS_2$
16 μm
13
1.05
1
0.074
0.053
255 MW/cm^2
30
IR$_{cutoff}$
SHG
Δn
LDT

Poster Presentation : **INOR.P-140**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Synthesis of Stability Enhanced Multi-Shelled InP/ZnSeS/ZnS Quantum Dots through Surface Treatment with Hafnium Butoxide

Seonwoo Ahn, 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*

Because of their properties of environmentally friendliness and narrow full width at half of maximum (FWHM), InP-based quantum dots (QD) are a promising material for light-emitting applications. However, to apply InP QD to down-converted light-emitting diodes (DC-LEDs), it is necessary to enhance their stability against harsh environments, such as those involving high temperature and strong irradiation of light. Therefore, we introduced a simple and effective strategy for enhancing the stability of QDs via passivation of their surfaces with hafnium butoxide [Hf(OtBu)4]. Green InP/ZnSeS/ZnS QDs were prepared using a hot-injection method and the QD surfaces were passivated by injection of Hf(OtBu)4 during synthesis. The stabilities of pristine and Hf(OtBu)4 treated QD solutions were compared during UV irradiation and thermal exposure. As a result, since the presence of Hf(OtBu)4 protected the surface of QD from damage, it was revealed that Hf(OtBu)4 treatment is effective at enhancing colloidal QD stability.

Poster Presentation : **INOR.P-141**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Regioisomerism of Functional Groups in Metal-Organic Frameworks

Dopil Kim, Hyeon Bin Ha, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

One of the major advantages of metal-organic frameworks (MOFs) are relatively easy functionalization with chemical tags. Both pre-functional group loadings and post-synthetic modifications are powerful methods to introducing various organic functional groups into MOF pores, and this unique functional groups allow the additional properties onto porous MOFs such as selective separation, efficient catalysis and molecular storages.

From 2011, our group have focused on the site-selective functionalization on MOFs with useful organic functional groups.[1] A variety of functional group combinations are intensively studied with regioisomeric installation into several MOF systems, and the relationship between the position of functional groups and structural features has been investigated with pillared MOFs. The structural flexibility of MOFs was directly related with regioisomerism of functional groups.[2,3]

In this presentation, we will discuss our recent results for functional group regioisomerism in MOFs for their property changes. The combination of functional group, physical mixture, structural changes along with computational studies will be presented and summarized.[4,5]

References

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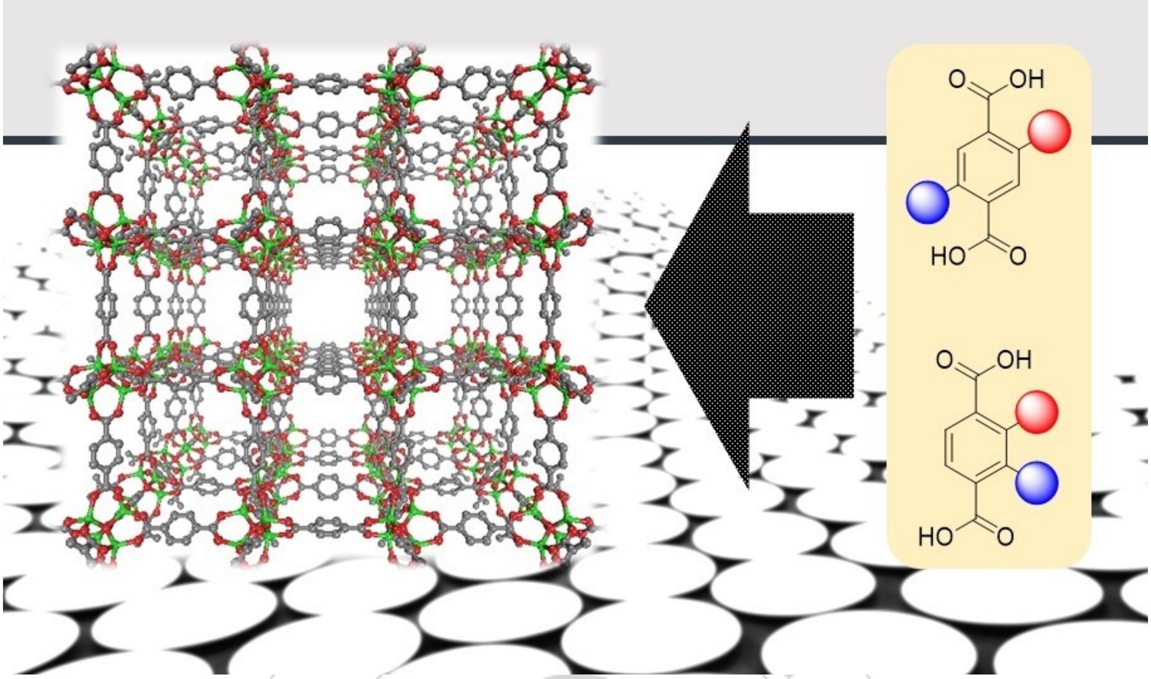

Poster Presentation : **INOR.P-142**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Removing MOF Oxidation Catalysts from the Reaction Media for the Further Oxidation Reactions

Ha-Eun Lee, Seongwoo Kim, Mi Hee Lim[1], Min Kim*

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

Metal-Organic Framework (MOFs) are emerging catalytic platform for various organic transformations due to their unique metal-ligand combination and useful porosity. Recently, the selective aerobic oxidation of benzyl alcohols to corresponding aldehydes have been extensively studied with functionalized MOFs. Both metal-decoration and organic oxidation functionalizations were studied within MOF pores for aerobic oxidation catalysts. However, the further oxidation of aldehydes to carboxylic acids is still challenging with MOF catalyst due to the produced carboxylic acids (additional binding, pore-blocking, catalyst poisoning, and etc).

Herein, our recent efforts for a selective conversion of alcohols to carboxylic acids using TEMPO-functionalized MOFs will be presented. The TEMPO-functionalized MOFs are a good catalytic platform for the aerobic oxidation of alcohols to aldehydes.[1,2] Overoxidized, carboxylic acid was not detected at all for the aerobic oxidation. The second oxidation of aldehyde to carboxylic acid was performed through the auto-oxidation. The conversion of alcohol to aldehyde was not occurred under the auto-oxidation condition. Under this mechanistic understanding, the removal process of MOF catalyst for the reaction media was attempted, and the selective efficient conversion of alcohols to corresponding carboxylic acids have been achieved. The detail development along with mechanistic control experiment will be discussed.

References

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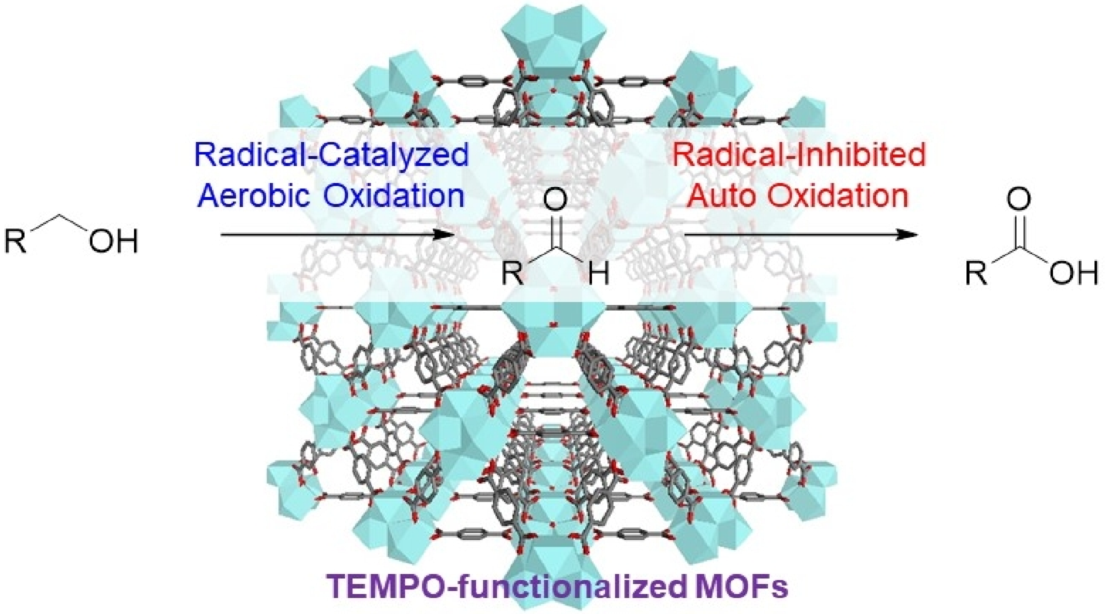
R OH
Radical-Catalyzed
Aerobic Oxidation
O
R H
Radical-Inhibited
Auto Oxidation
O
R OH
TEMPO-functionalized MOFs

Poster Presentation : **INOR.P-143**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Thiol-Ene Click Chemistry for Efficient Methods for MOF-MMM Composite Preparation with Controlled Functionalities

Jooyeon Lee, Min Kim*

Department of Chemistry, Chungbuk National University, Korea

Metal-Organic Frameworks (MOFs) are emerging 3-dimentional porous materials for various application by utilizing their unique pore environment. Although MOFs have many interesting features, their relatively unstable nature to polar conditions restrict real application under industrial level. Therefore, the hybrid composite materials between MOFs and polymeric mixed-matrix membranes have been widely studied. Generally, simple blending methods were employed for preparing the composite materials. Recently, the covalent connection between MOFs and MMMs for interfacial controls.

Recently, we have successfully demonstrated that the efficient covalent bond connection between MOF-MMM using 'Thiol-ene photo click reaction'. We could load up to 60 wt% MOFs in this composite material.[1] In addition, the additional functional group controls have been achieved in this MOF-MMM composite materials through post-synthetic ligand exchange (PSE) technique.[2] The core-shell structure from PSE was employed, and the core functionality was controlled in MOF-MMM for pore size and polarity changes. At the same time, the shell part with vinyl group was fully utilized for thiol-ene click chemistry. The detail strategy along with preparation of materials and characterization will be discussed. The control of pore functionality in MOF-MMM was applied to gas separation experiment.

Reference

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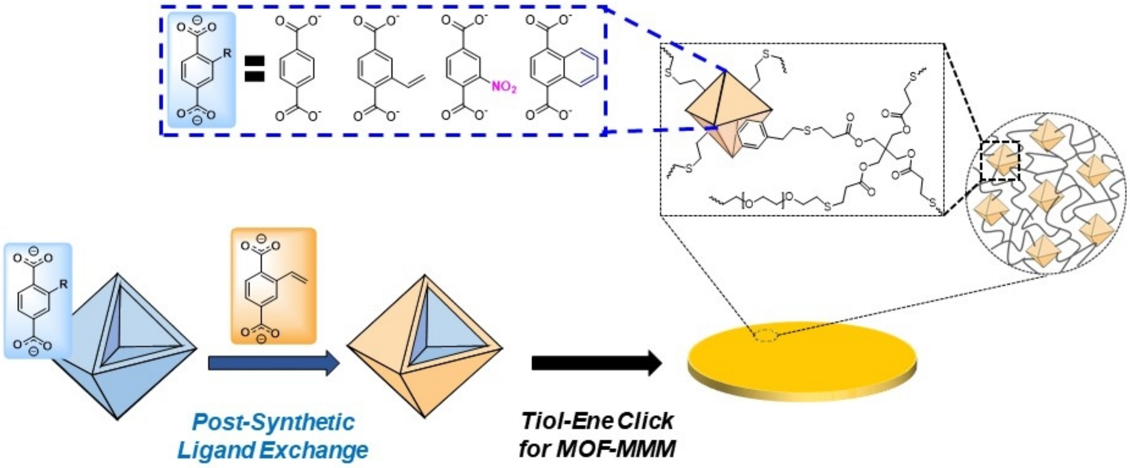
R
=
NO2
Post-Synthetic
Ligand Exchange
Tiol-Ene Click
for MOF-MMM

Poster Presentation : **INOR.P-144**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Enhanced Stability of Copper Indium Sulfide Quantum Dots by Doping Aluminum into the ZnS Shell

Seo yeon Shin, Minji Ko, Young rag Do*

Department of Chemistry, Kookmin University, Korea

In this study, to improve the stability of QDs, aluminum doped Cu-In-S/ZnS (CIS/ZnS) quantum dots (QDs) were synthesized using hot-injection method. This red emissive Al-doped CIS/ZnS QDs showed an excellent photoluminescence quantum yield (PLQY) of over 80%. To compare the stability of Al-doped CIS/ZnS QDs, pristine CIS/ZnS QDs were prepared. The two types of QDs were subjected to continuous UV irradiation and to heat for 18 hours, respectively. The pristine QDs, which were irradiated and heated for a period, showed efficiencies of 31% and 14%, respectively, compared to the initial efficiencies of the QDs. On the other hand, the Al-doped QDs showed efficiencies of 70% and 74%, respectively, compared to the initial efficiencies after the same stability test. As a result, the excellent stability of Al-doped QDs was confirmed by comparison with values of pristine QDs.

Poster Presentation : **INOR.P-145**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Variation of Optical Characteristic and Diameter of InGaN/GaN Nanorods by KOH Treatment Time

Selim Yun, Gang Yeol Yoo[1], Woong Kim[2,*], Young rag Do[3,*]

Department of Chemistry , Kookmin University, Korea
[1]*Department of Advanced Materials Engineering, Korea University, Korea*
[2]*Division of Advanced Materials Engineering, Korea University, Korea*
[3]*Department of Bionano Chemistry, Kookmin University, Korea*

We fabricated InGaN/GaN nanorods from epitaxially grown substrate with a light-emitting diode (LED) structure by top-down process using an inductively coupled plasma (ICP) etching process. However, the high-energy plasma induced physical damage on the nanorod surface when the GaN layer was used to etch rod-shapes; also, the optical characteristic of the GaN nanorods declined. In this study, we performed KOH treatment for 40 min to remove plasma-induced surface damage of nanorods with diameter of 630 nm. Compared to the as-etched materials, we confirmed through scanning electron microscopy (SEM) that the nanorod shape changed as the nanorod diameter decreased by 200 nm when KOH treatment was performed. In addition, photoluminescence (PL) intensity of the peak wavelength of 440 nm increased as the proportion of defect peaks that appeared as surface defects decreased through low-temperature PL. Therefore, we confirmed that KOH treatment of GaN nanorods removed surface defects and improved optical properties.

Poster Presentation : **INOR.P-146**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Fabrication of Patterned Molybdenum via Nanoimprint Lithography using Spin-on-Glass as Imprint Resin

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applied chemistry, Kookmin University, Korea
[1]*Department of Chemistry, Kookmin University, Korea*
[2]*Department of Bionano Chemistry, Kookmin University, Korea*

There are several practical methods, such as polystyrene (PS)-based nanosphere lithography (NSL), electron beam lithography (EBL) and nanoimprint lithography (NIL), that can be used to fabricate nano-patterns. For mass production, NIL is more suitable than PS-NSL; NIL is competitive in price relative to EBL. For this reason, research on nanometer scale patterning using NIL, a technology that including stamps and templates, has drawn attention. NIL is a simple technique that adjusts the template and deposition it on the substrate using imprint resin. Nanoimprinting- using spin-on-glass as an imprint resin is a technology that involves no separate heating or UV-exposure. A spin coating technique of spin-on-glass on polydimethylsiloxane (PDMS), a material of soft stamps, was carried out for nanometer scale patterning. Using this method, a molybdenum (Mo) layer, which material is mostly used as a back-electrode of CIGS solar, was directly patterned with a diameter of 550 nm, a depth of 650 nm and a period of 1.2 ㎛. As a result of using a patterned MO electrode, the efficiency of CIGS solar cells can be expected to improve due to increases in surface area on which excitons are separated and decreases in distance between the p-n junction and the electrode.

Poster Presentation : **INOR.P-147**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

Conjugated microporous polymer synthesized by one building block: Enhancement of catalytic performance for biomass conversion

Kyoungil Cho, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

The conjugated microporous polymer (CMP) was synthesized by Sonogashira reaction of one building block for terminal alkyne rich material which can be modified various functional catalysts.[1] One building block was prepared by 1,4-diethynyl-2,5-dibromobenzne. Silica was used as a template with an average diameter of 250nm to create a hollow form.[2] After etching the silica template by hydrogen fluoric acid, the shell thickness of the synthesized H-TA-CMP was 20-25nm. We used enriched terminal alkyne polymer as a control system which was synthesized by Sonogashira reaction of 1,3,5-triethynylbenzene and 1,4-dibromobenzene. Aliphatic sulfonic acid was introduced in H-TA-CMP by thiol-yne reaction to produce H-TA-CMP-ASO$_3$H. As another control system, H-control-SO$_3$H was prepared by aromatic sulfonic acids with H-TA-CMP. H-TA-CMP-ASO$_3$H showed high 5-hydroxymethylfurfural (HMF) yield over 90 % in reaction of D-fructose to HMF. During 5 recycle reactions, H-TA-CMP-ASO$_3$H showed 90% of yield, however, H-control-SO$_3$H showed declining yield over the cycles. References 1. K. Cho, S. M. Lee, H. J. Kim, Y. J. Ko and S. U. Son. *J. Mater. Chem. A*, 2018, 6, 15553.2. N. Kang, J. H. Pack, M. Jin, N. Park, S. M. Lee, H. J. Kim, J. M. Kim and S. U. Son. *J. Am. Chem. Soc.*, 2013, 135, 19115

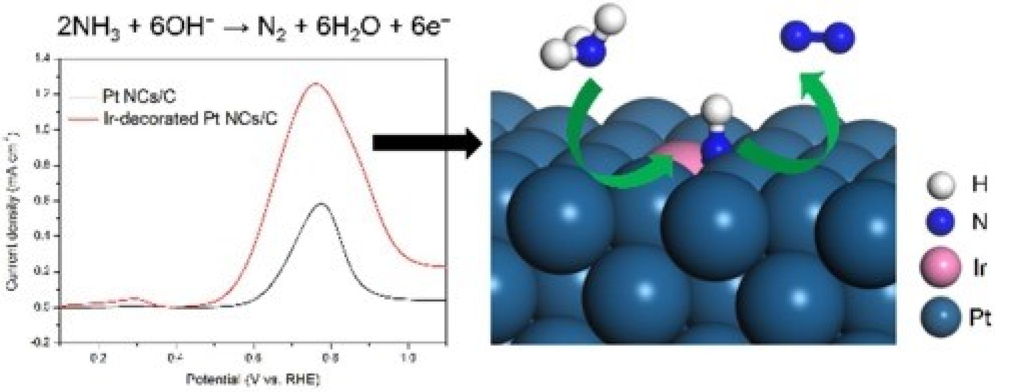
Poster Presentation : **INOR.P-148**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Surface Engineering of Pt Nanocubes towards the Ammonia Electrooxidation Reaction

Hye Jin Lee, Kumar Siddharth[1], Xueping Qin[1], Sang-Il Choi[*], Minhua Shao[1,*]

Department of Chemistry, Kyungpook National University, Korea
[1]*Department of Chemical and Biological Engineering, The Hong Kong University of Science and Technology, Hong Kong, Hong Kong*

Ammonia (NH_3) electro-oxidation reaction (AOR) has attracted much attention in recent years as an important reaction in direct NH_3 fuel cells, wastewater remediation, and NH_3 electrolyzer. However, sluggish reaction kinetics and its structure-sensitive properties require specific designs of advanced catalysts to achieve optimized performance. This presentation reports Ir-decorated Pt nanocubes and Ir and $Ni(OH)_2$-decorated Pt nanocubes are developed as unique surface engineered model catalysts. The surface-decorated Ir and $Ni(OH)_2$ on the Pt nanocube were confirmed by a number of technique, including energy-dispersive X-ray spectroscopy mapping, X-ray diffraction, and X-ray photoelectron spectroscopy. The electrochemical measurement results of Ir-decorated Pt nanocubes showed 2.15 times higher AOR activity than commercial Pt/C. Then, Ir and $Ni(OH)_2$-decorated Pt nanocubes showed great stability during AOR measurement. And theoretical simulation results also presented for demonstrating surface engineering effects of Ir and $Ni(OH)_2$ toward the AOR.



Poster Presentation : **INOR.P-149**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

Microporous Organic Polymer Bearing Fe_3O_4 Nanoparticles: Multi-Functional Drug Delivery Systems with Targeting, Imaging, and Magneto-Thermal Behaviors

June Young Jang, **Seung Uk Son**[*]

Department of Chemistry, Sungkyunkwan University, Korea

Microporous Organic Polymer Bearing Fe_3O_4 Nanoparticles: Multi-Functional Drug Delivery Systems with Targeting, Imaging, and Magneto-Thermal Behaviors Microporous organic polymers (MOPs) have attracted significant attention of scientists as a new class of porous materials. Due to their high surface areas and chemical stability, the MOPs have been applied to various fields such as adsorbents, catalysts, and energy storage materials. However, the application of MOP to bio-fields is in its early stage. This work shows a designed synthesis of MOP-based drug delivery systems. This work shows that multifunctional drug delivery materials could be developed by the combination of functional inorganic nanomaterials with MOP chemistry. The Fe_3O_4@Void@MOP-TE-FA exhibited folate receptor targeting for cancer cells, aggregation-induced emission-based imaging ability, DOX drug delivery, and magneto-thermal properties, eliciting the efficient antitumor effect by the combined chemotherapy and hyperthermal-therapy. We believe that more various multifunctional drug delivery systems can be designed by the combination of inorganic nanomaterials with MOP materials and by the combination of pre-designed building block approach with the post-synthetic modification strategy.

Poster Presentation : **INOR.P-150**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Dynamic Self-Assembly of Sublimable Caffeine in the Covalent Formation of Microporous Organic Polymer for Morphology Evolution and Enhanced Performance

Chang Wan Kang, Seung Uk Son[*]

Department of Chemistry, Sungkyunkwan University, Korea

This work shows that the morphology of microporous organic polymer (MOP) can be controlled via dynamic self-assembly of sublimable caffeine in the covalent formation. Because the functional performance of MOP is dependent on its morphological structure, Thus, the shape-controlled synthesis of MOP materials is important. Caffeine is one of the most common compounds in daily life, and the chemical and physical behaviors of caffeine have been a popular research subject for the last several decades. In poor solvents, it readily forms self-assembled aggregates through intermolecular interaction. The aggregates usually show 1D outer morphologies such as wires, rods, and needles. The intermolecular forces between caffeine molecules are not so strong, making the solid aggregates of caffeine sublimable. In our own studies, we discovered that the molecular assembly behaviors of caffeine are dynamic. When we added caffeine to triethylamine, precipitates immediately formed, showing morphologies of short rods. When we stirred the precipitate suspension in triethylamine at 90 °C, the lengths of rods were elongated to wires with a gradual decrease of thicknesses. In the presence of caffeine, the MOP showed 1D shape evolution, templating the *in situ* dynamically self-assembled caffeine. Through the control of experimental conditions, the ribbon-like and tubular MOP materials could be engineered. The shape-controlled MOP materials showed striking benefits such as sharply enhanced sensing of harmful compounds and enhanced catalytic performance in the CO_2 fixation, due to the reduced diffusion pathways of guests. We believe that the "*caffeine method*" in this work can be applied to more various MOPs.

Poster Presentation : **INOR.P-151**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

NSelf-Supported Pd Nanocatalysts in the Formation of Stille Coupling-Based Microporous Organic Polymers for Visible Light-Driven Suzuki ReactionsN

Sang Hyun Ryu, Seung Uk Son*

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This work shows that the Stille coupling reaction provides interesting MOP chemistry.Recently, visible light has been recognized as a sustainable energy source not only in the generation of electricity but also in organic synthesis. Visible light-induced cross-coupling by the combination of Pd catalysts with visible light-harvesting materials has been an important research subject.In this work, first, we discovered that Pd nanocatalysts (1~3 nm) were self-supported in the St-MOP to form St-MOP@Pd via one pot synthesis. The amount of Pd nanocatalysts in the St-MOP@Pd could be controlled by Pd catalysts.Recently, microporous organic polymers (MOPs) have been prepared by Pd-catalyzed cross-coupling reactions. It is noteworthy that the Stille coupling doesn't require additional bases. In this work, we report the Stille coupling-based MOP materials (St-MOP), showing that the Stille coupling can supply chemistry in the MOP materials.Second, we discovered interesting growth principles of the St-MOP. The size of St-MOP particles was sensitive to the amount of Pd catalysts and could be systematically controlled. Third, the St-MOP materials in this work were visible light active. The St-MOP@Pd showed excellent photocatalytic performance in the visible light-driven Suzuki coupling. Among the St-MOP@Pd materials(St-MOP@Pd-1, St-MOP@Pd-2, St-MOP@Pd-3), St-MOP@Pd-2 with an optimal amount of St-MOP and Pd NPs showed efficient photocatalytic activities in the visible light-driven Suzuki– Miyaura coupling.This work shows that the Stille coupling reaction provides interesting MOP chemistry. The St- MOP showed visible light absorption at 450 nm and emission at 522 nm. The emission was quenched by Pd NPs, indicating efficient visible light-induced electron transfer from St-MOP to Pd NPs. the optimal St-MOP@Pd-2 (0.14 mol% Pd) showed a TON of 657 and a TOF of 219 h-^{2}1^{2} in the visible light-driven Suzuki coupling of 1-acetyl-4-bromobenzene and phenyl boronic acid at 25o^{2}C. The highly efficient photocatalytic performance of St-MOP@Pd-2 is attributable to its harmony between visible light-harvesting material (St-MOP) and Pd NPs.

Poster Presentation : **INOR.P-152**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

Comparison of Breakdown Voltage Point According to Atomic-Layer-Deposited Passivation Materials and Optimization of Size and Thickness of the Passivation Area

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[1]*Department of Bionano Chemistry, Kookmin University, Korea*

To study the tendency of breakdown voltage according to passivation materials, the metal-insulator-metal (M-I-M) structure was fabricated. ITO and Ti were deposited by sputter and E-beam evaporator, respectively, as bottom and top contact pad. The passivation material, which was located between top and bottom contact pad, were selected from HfO_2, ZrO_2, and Al_2O_3, and the deposition of passivation material was carried out by atomic-layer-deposition (ALD). By using a probe station to measure a current-voltage (I-V) curve from -40 V to 0 V, we derived that different passivation materials have different breakdown voltage trends under identical thickness of passivation materials, and in this study, Al_2O_3 had the highest breakdown voltage of 12 V. Based on this result, we choose Al_2O_3 for passivation material in order to research size and thickness effects. Through subsequent experiments the conclusion is drawn that leakage current can be reduced by increasing the breakdown voltage which results from choosing a passivation material, size and thickness of that.

Poster Presentation : **INOR.P-153**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

Investigation of Li^+/H^+ Ion Exchange on the Fast Lithium Ion Conductor, $LiTa_2PO_8$

Gunwoo Yoo, Jaegyeom Kim, Seung-Joo Kim*

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The ion-exchange properties of various solid lithium ion electrolytes have been explored. Particularly, the substitution of protons for lithium ions has been attracted due to their potential application for solid state proton exchange membrane fuel cells. In this study, a new protonated compound, HTa_2PO_8, was successfully synthesized via the ion-exchange reaction of $LiTa_2PO_8$. Crystal structure of deuterium substituted DTa_2PO_8 was determined by the complementary use of synchrotron X-ray powder diffraction (SXPD) and neutron powder diffraction (NPD). The impedance measurements under dry air, wet air, and wet 5% H_2/Ar conditions revealed that the main transporting species is proton in HTa_2PO_8. The compound exhibited good proton conductivity: c.a. 2×10^{-6} S cm^{-1} at 300 °C, which is superior to those of protonated NASICON–type compounds. TG-DSC and HT-XRD analyses show that the HTa_2PO_8 decomposes through two steps: $HTa_2PO_8 \rightarrow Ta_2PO_{7.5}$ (T ≈ 600 °C) → 1/2 $Ta_2O_5 + TaPO_5$ (T ≈ 1050 °C).

Poster Presentation : **INOR.P-154**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

Synthesis, structure determination, and characterization of a new centrosymmetric strontium niobium oxyfluoride

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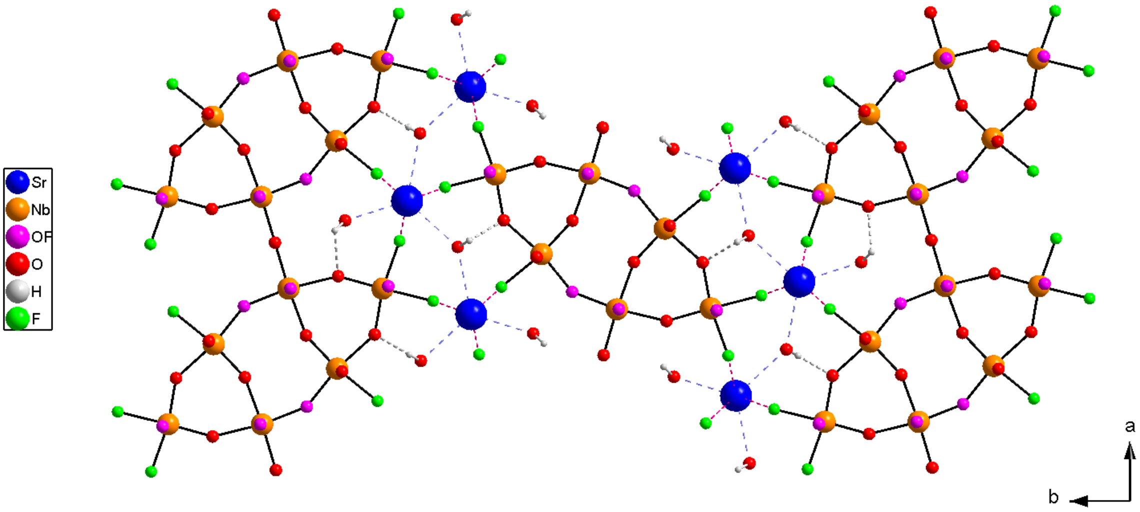
[1]*Department of Chemistry, Sogang University, Korea*

A new strontium niobium oxyfluoride compound has been synthesized by a hydrothermal reaction. Single crystal X-ray diffraction indicates that the title compound possesses the centrosymmetric space group, *Pbam*. The crystal structure of the title compound features a layered structure composed of a $Nb_3O_6F_3(OF)_6$ moiety. This moiety is composed of $Nb(1)O_2F_2(OF)_2$, $Nb(2)O_4F(OF)$, and $Nb(3)O_3(OF)_3$ octahedra, which share corners through O atoms to form a $Nb_3O_6F_3(OF)_6$ ring. Sr^{2+} and H_2O are located between the layers. Sr^{2+} cations are coordinated with the neighboring fluorine atoms and water molecules to form a tricapped trigonal prism geometry. A more detailed structural analysis indicates that strong hydrogen bonding interactions between oxygen anions and water molecules exist. Thus, the material can be considered as a two-dimensional layered structure. A complete characterization such as thermal, elemental, and spectroscopic analyses will be also provided.


Sr
Nb
OF
O
H
F
a
b

Poster Presentation : **INOR.P-155**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

Nanoparticulate Conjugated Microporous Polymer with Post-Modified Benzils for Enhanced Pseudocapacitor Performance

So Young Park, Seung Uk Son*

Department of Chemistry, Sungkyunkwan University, Korea

Conjugated microporous polymers (CMPs) are recent and versatile functional materials. Due to the conjugated chemical structure of CMPs, the CMPs have been explored as charge storage materials. However, new ideas and more efforts are required to enhance the electrochemical performances of CMPs. This work shows a new smart way for enhancing CMPs to be redox active; 1) nanoparticulation and 2) $FeCl_3$-catalyzed post-modification of diaryl alkyne moieties in the CMPs to the redox active benzil moieties. The redox activity of molecular benzil was demonstrated by the model studies. Recently, pseudocapacitive materials have attracted considerable attention from scientists to improve the capacitances with the help of additional redox species in the materials. In our study, we fabricated symmetric coin cell type two-electrode pseudocapacitors. Nanoparticulate CMP (N-CMP) with an average diameter of 41 ± 4 nm was prepared through the kinetic growth control in the Sonogashira coupling of 1,3,5-triethynylbenzene with 1,4-diiodobzene. The N-CMP is rich of a diphenylacetylene moiety in its chemical structure. The nanoparticulate CMP with post-modified benzils (N-CMP-BZ) showed distinct enhancement of electrochemical performance, compared to the model material, CMP, CMP-BZ and N-CMP. With the help of the pseudocapacitive behavior of N-CMP-BZ, the capacitances and conductivities of materials were significantly improved. The excellent electrochemical performance of N-CMP-BZ is attributable to the enhanced utilization of functional sites by a nanosize effect and the additional redox contribution of benzil moieties.

Poster Presentation : **INOR.P-156**
Inorganic Chemistry
Zoom 2 WED 17:30~18:00

PET@microporous organic polymer@Cu films: flexible and metal-economical electromagnetic interference shielding materials

Seong In Park, Seung Uk Son*

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As various electric devices have been extensively generalized, electromagnetic radiation (EM) pollution has become an important issue. This work shows that microporous organic polymer (MOP) chemistry can be applied for the engineering of electromagnetic interference shielding membranes. With the help of thin MOP coating with microporosity and coordinative functionality, flexible and metal-economical Cu-polymer composite films could be realized. In this work, we report the coating of polyethylene terephthalate (PET) fibers with MOP with amino groups (MOP-A), the adsorption of Ag+, and Ag-catalyzed electroless deposition of copper into the PET@MOP-A films. It is noteworthy that bulk Cu (100wt%) with a thickness of 10 µm showed EMI shielding ability of 70 dB against EM of 8.2~12.4 GHz (X-band) in the literature. Considering 41wt% Cu with a thickness of 0.64 µm in the PET@MOP-A@Cu-40, the observed EMI shielding performance (64.3~73.8 dB against EM of 7.5~12 GHz) indicates the efficient use of Cu. Moreover the PET@MOP-A@Cu showed excellent EMI shielding performance and performance retention against 1000 bending (R = 5 mm) numbers.

Poster Presentation : **INOR.P-157**

Inorganic Chemistry

Zoom 2 WED 17:30~18:00

Development of Simple Non-Visual Illuminance to Estimate Melatonin Suppression

Yun Jae Eo, Keyong Nam Lee, Young rag Do*

Department of Chemistry, Kookmin University, Korea

Since indiscriminate and inadequate artificial lighting can affect our circadian rhythms, we should consider not only the efficiency of artificial lighting but also its effects on human health. Especially, it is known that melatonin hormone, which is related to the circadian rhythms, is regulated by non-visual illuminance (NVIL), not visual illuminance (VIL). However, it is difficult to find a simple dosimeter that can easily measure NVIL. Therefore, we fabricated an illuminometer that can measure both NVIL and VIL, using optical filters mimicked action spectra, such as melanopic action spectrum and photopic spectral luminous efficiency function, according to new standard of the Commission Internationale de l'Eclairage (CIE). In addition, we estimated the degree to which melatonin could be suppressed depending on the NVIL. Accordingly, using this simple illuminometer, we will be able to maintain our circadian rhythms by adjusting the light environment as needed.

Poster Presentation : **INOR.P-78**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Stable Cu(II) and Cu(I) complexes with a same ligand

Eun su Chae, Jang Hoon Cho, Hong In Lee*

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Selective primary alcohol oxidation is continuously attracting attention due to the productions of aldehydes and carboxylic acids. One of the eco-friendly primary alcohol oxidation method is using a copper-containing fungal enzyme called GOase (galactose oxidase), which can oxidize primary alcohol at aerobic condition. Inspired by this enzyme, several N_2O_2 or N_4 copper complexes that can oxidize alcohols were reported by mimicking the active site of GOase. During GOase-like alcohol oxidation, copper changes its valent from Cu(II) state to Cu(I) state. To understand the reactions of GOase-like alcohol oxidations of copper complexes, we have tried to synthesize stable Cu(II) and Cu(I) complexes with a same ligand. In this study, we have synthesized a new ligand EbQMA (=(N*E*,N'*E*)-2,2'-(ethane-1,2-diyl)bis(N-(quinolin-8-ylmethylene)aniline)), to develop stale copper complexes, [Cu(I)(EbQMA)]ClO_4 and [Cu(II)(EbQMA)]$(ClO_4)_2$, in aerobic condition. Evidences for changing copper valent in alcohol was monitored by NMR spectroscopy.

Poster Presentation : **INOR.P-79**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Redox-Inactive Metal Ions Enhance the Nucleophilic Reactivity of an Alkylperoxocopper(II) Complex

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

The importance of redox-inactive metal ions in modulating the reactivity of redox-active biological systems is the subject of great current interest. In this work, the effect of redox-inactive metal ions ($M^{3+} = Sc^{3+}$, Y^{3+}, Yb^{3+} and La^{3+}) on the nucleophilic reactivity of a mononuclear ligand-based alkylperoxocopper(II) complex, $[Cu(^{i}Pr_2\text{-tren-}C(CH_3)_2O_2)]^+$ (**1**), was examined. **1** was prepared by addition of H_2O_2 and triethylamine to the solution of $[Cu(^{i}Pr_3\text{-tren})(CH_3CN)]^+$ ($^{i}Pr_3$-tren = tris[2-(isopropylamino)ethyl]amine) via the formation of $[Cu(^{i}Pr_3\text{-tren})(OOH)]+$ (**2**) in CH_3OH at 30 °C. **1** was characterized using DFT calculations and spectroscopic methods such as UV-vis, rRaman and EPR. DFT calculations support the electronic structure of **1** with an intermediate geometry between trigonal bipyramidal and square pyramidal geometry, which is consistent with the observed EPR signal exhibiting a signal. The reactivity of **1** was investigated in oxidative nucleophilic reactions. The positive slop of Hammett plot ($\rho = 2.3(1)$) with *para*-substituted benzaldehydes and the reactivity order with 1°-, 2°-, 3°-CHO demonstrate well the nucleophilic character of this Cu(II) ligand-based alkylperoxo complex. Lewis acidity of M^{3+} improves the oxidizing ability of **1**. The modulated reactivity of **1** with M^{3+} was revealed to be an opposite trend of the Lewis acidity of M^{3+} in aldehyde deformylation.

Poster Presentation : **INOR.P-80**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Hybridizing of metal organic framework in selectively modified clay nanotube for enhanced gas adsorption capacity

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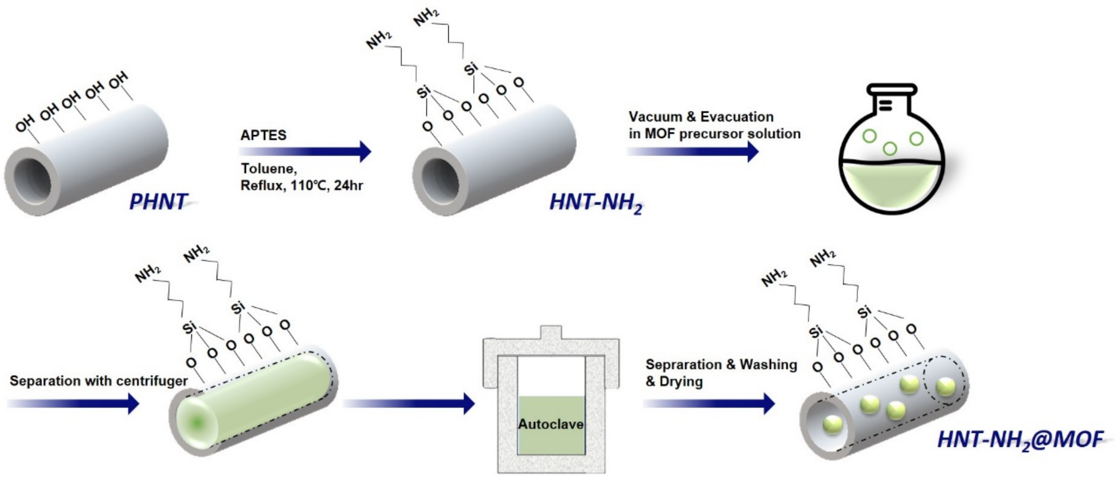
[1]*Department of Chemistry, Hanyang University, Korea*

Metal organic frameworks (MOFs) are hybrid materials that consist of organic ligands and metal ions or clusters. Increasing number of MOFs have recently been recognized for a great potential in CO2 capture due to their high surface area. Especially, HKUST-1 consisted of copper nodes and organic ligands is one of the most widely studied MOFs owing to its high porosity. In this work, we synthesized HKUST-1 in the lumen of modified Halloysite clay nanotubes (mHNTs). Firstly, inner or outer surface of HNTs were selectively modified with sulfuric acid and (3-Aminopropyl)triethoxysilane. Each mHNT was designated EHNT and HNT-NH2. Then, HKUST-1 precursor was evenly loaded into the lumen of HNTs in a solution phase, and the crystalline MOFs were syntehsized via solvothermal method. The final procuct was named to EHNT@HKUST-1, HNT-NH2@HKUST-1 respectively.By confining space inside the nanotube, HNTs acted as a nanocarrier to make specific boundary for growing MOFs with longitudinal axis of HNTs and enhance water stabililty of MOFs. Also, selectively modified HNTs imparted unique properties to the surface of composites. Gas adsorption capacity was analyzed by Brunauer-Emmett-Teller (BET) using N2 and CO2 gases. Specifically, 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 cm3(STP)g-1 to 19.332 cm3(STP)g-1. Additionally, HNT-NH2@HKUST-1 indicated around 24.849 cm3(STP)g-1 of CO2 gas adsorption capacity. These nanocomposites were analyzed by SEM, TEM-EDS and XRD in an effort to investigate the morphological and structural characteristics. This work can be a trigger to synthesize various hybrid nanotube materials for synergistic effects and applied to competitive adsorbents for gas capturing.


OH OH OH OH OH
PHNT
APTES
Toluene,
Reflux, 110℃, 24hr
NH2
NH2
Si
Si
O O O O O O O
HNT-NH2
Vacuum & Evacuation
in MOF precursor solution
Separation with centrifuger
Autoclave
Sepraration & Washing
& Drying
HNT-NH2@MOF

Poster Presentation : **INOR.P-81**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Assembled nanoparticles on the polymeric template for enhancement of physical properties

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Nanomaterial exhibits varying physical properties alongside with morphological and dimensional differences. One of the essential characteristics of magnetic nanoparticle (MNP), the superparamagnetism is derived from the point of reduction to nano-level. Other nanomaterial properties called surface plasmonic resonance effect represent unique traits of gold nanoparticle (AuNP) and magneto plasmonic nanoparticle (MPN). However, controlling the magnetism and plasmonic effect requires a lot of efforts such as replacing material, dopping additional elements, and growth of nano-shell from the given material. Here, by simply performing surface modification and chemistry-based assembly, magnetism and plasmonic effects are altered significantly regardless of nano-scale change. Template-based chemical assembly (TBCA) enables potential to increase in saturation magnetization while maintaining superparamagnetism and induced minute plasmonic resonance peak control. Template used in TBCA comprising polystyrene polymer beads barely hinders magnetism and plasmonic effect, yet successfully becomes substrate form TBCA process. Also, with fast copper-free click chemistry, the TBCA provides the noteworthy potential to be applied in biomedical engineering by reducing cytotoxicity and fast-reliable reaction.

Poster Presentation : **INOR.P-82**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Various pathways for synthesis of BaSi2O2N2:Eu2+ phosphors from silicate phosphors

Kangsik Choi, Younbong Park[*]

Department of Chemistry, Chungnam National University, Korea

Oxy-nitride phosphors have been reported to have high luminescence intensities and thermal stability in white light LED applications. Among them, BaSi2O2N2:Eu2+ phosphor is a bluish green phosphor, which is applied to white LEDs with high CRI values. The method of improving the manufacturing process and characteristics of that phosphor is currently being actively studied. In this study, Ba2SiO4:Eu2+, Ba3SiO5:Eu2+ and Ba3MgSi2O8:Eu2+ phosphors were used as raw materials to synthesize BaSi2O2N2:Eu2+ phosphors. A silicate phosphor was mixed with Si3N4 and calcined in a reducing atmosphere to synthesize a final product. The BaSi2O2N2:Eu2+ phosphor was investigated by X-ray diffraction spectroscopy, scanning electron microscopy, photoluminescence analysis and temperature dependent photoluminescence. When Ba3MgSi2O8:Eu2+ phosphor was used as a raw material, the ratio of thermal quenching effect was the lowest. It is explained that local distortion caused by Eu2+ was relaxed by Mg2+ in the BaSi2O2N2:Eu2+ structure. As a result, we found that BaSi2O2N2:Eu2+ phosphors with high thermal stability could be a good candidate for white LED applications.

Poster Presentation : **INOR.P-83**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Electron Injection Process of Porphyrin Dye into Heterogeneous TiO_2/Re(I) Photocatalyst

Daehan Lee, Min Su Choe, Changhyun Back, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

The net hetero-collisional electron transfer from the non-anchored fluorescent porphyrin sensitizer to the TiO_2 catalytic particles was a major event during the initial stage of the catalysis. According to *in situ* UV–Vis absorption spectroscopy and mass analysis of dye solution filtered after photolysis, the initially added porphyrin dye experienced a significant photodegradation accompanied by a breakage of π–conjugation and loss of the bulky substituents. Acetyl- or ethyl-group modified porphyrins were prepared, respectively referred to as **ZnP**$_{\mathbf{Acet}}$ and **ZnP**$_{\mathbf{Et}}$, and this modification elevated the corresponding excited-state energy levels when comparing **ZnP** with **ZnP**$_{\mathbf{Et}}$, consequently shortening the activity delay at the early stage of photolysis. Thus, chemical modification had a favorable effect on the photosensitizing and electron transportation abilities of the dye.

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

High Selective and Efficient Photoconversion of Carbon Dioxide to Formate by New Mononuclear Nickel Complexes

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

Two mononuclear nickel Ni(II) complexes of pyridylbenzimidazole (pbi) and pyridylbenzothiazole (pbt) were prepared. The two Ni complexes were examined for CO2 conversion using eosin Y as a photosensitizer and triethanolamine as a sacrificial electron donor upon visible- light irradiation. Light-driven photoreduction of CO2 catalyzed by Ni(pbt)(pyS)2 and Ni(pbi)(pyS)2 (pyS = pyridine-2-thiolate) selectively affords formate with a a high efficiency and a high catalytic selectivity of ~99 %. The pbi complex exhibited a slightly faster rate and higher yield for the formate production than the pbt complex. Hydrogen production and kinetic isotope effects in the photocatalytic reactions with these Ni catalysts are also presented in relation to the CO2 reduction mechanism. These catalysts are the first examples of early transition metal complexes affording such high selectivity and efficiencies.

Poster Presentation : **INOR.P-85**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Photochemical CO_2 to CO/$HCOO^-$ Conversion by TiO_2-Immobilized $[Ru(bpy)(CO)_2Cl_2]^{2+}$ Catalyst

Min Su Choe, Daehan Lee, Su-Won Na, Chul Hoon Kim, Dae won Cho, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Herein, we report the details of two photochemical models, mixed homogeneous system (IrPS + RuPE) and binary hybrid system (IrPS + TiO_2/RuP) for estimating the catalytic behavior of homogeneous and heterogenized mono(bipyridine) Ru(II) catalyst, respectively; IrPS is a heteroleptic Ir(III) complex, $[Ir(C^{\wedge}N)_2(N^{\wedge}N)]^+$ (C^N = 1-phenylisoquinoline; N^N = 4,4'-dimethyl-2,2'-bipyridine), RuPE is Ru(4,4'-Y_2-bpy)$(CO)_2Cl_2$ (Y = $CH_2PO(OEt)_2$), RuP is Ru(4,4'-Y_2-bpy)$(CO)_2Cl_2$ (Y = $CH_2PO(OH)_2$), and the sacrificial electron donor (ED) is 1,3-dimethyl-2-phenyl-1,3-dihydrobenzimidazole (BIH). A combined photolysis study and in situ FTIR analysis shows that the TiO_2 immobilization of molecular Ru(II) catalyst efficiently suppresses the polymerization of Ru(II) catalyst and leads to the dominant participation of monomeric and local dimeric mechanism of adsorbed Ru(II) catalyst, which are characterized respectively as 1) key monomeric intermediates ((bpy)RuI(OCHO)$(CO)_2$Cl and (bpy)RuI(COOH)$(CO)_2$X)) and 2) undefined Ru-Ru dimeric intermediates for CO and formate production mechanism, consequently resulting in the steady catalytic CO/formate production during prolonged photoreaction.

Poster Presentation : **INOR.P-86**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Rhodamine-based Near-Infrared Probe for Fluorescent Detection of ATP and Staining Lysosomes in Living Cells

Jinheung Kim

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

An important biomolecule, adenosine triphosphate (ATP) is found in all forms of living things and is considered as the molecular unit for intracellular currency transfer. Research has shown that the level of phosphate-containing metabolites can be utilized as a symptom of disorder or dysfunctions in biological systems. Thus, selective and real-time detection of ATP is imperative to biochemical studies and clinical diagnosis. A new near infrared fluorescent probe was designed and prepared to detect ATP and target lysosomes in cells. The non-fluorescent probe was turned on during the interaction with ATP, affording a 115-fold increase in fluorescence intensity. The colorless probe turned purple upon interaction with ATP. The probe displayed high sensitivity and selectivity toward ATP compared with other biomolecules, such as AMP, ADP, GMP, and CMP. Such significant spectroscopic changes derive from a structural change of the probe's spirocyclic moiety to its ring-opened form. This occurs through electrostatic and □,□-stacking interactions between the probe and ATP. This probe was also used in selective lysosome staining and for real-time ATP level monitoring. It exhibits great advantages in cell imaging studies, such as excellent photostability, low cytotoxicity, and good cell membrane permeability.

Poster Presentation : **INOR.P-87**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Highly Efficient Porphyrin-Driven CO_2 Reduction via Hetero-Collisional Electron Transfer Route between Homogeneous Porphyrin and TiO_2 Semiconductor.

Min Su Choe, Daehan Lee, Changhyun Back, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A zinc porphyrin complex (ZnP) was applied as visible-light photosensitizer in solution to the selective CO_2 reduction to CO in the presence of an electron donor (BIH) and a hybrid catalyst (TiO_2/ReC) prepared by anchoring of Re(4,4′-Y_2-bpy)$(CO)_3$Cl (Y = $CH_2PO(OH)_2$) on TiO_2 particles. LED irradiation in N,N-dimethylformamide (DMF) at >500 nm resulted in the successful reduction of CO_2 to CO. The systems efficiently proceeded CO_2 to CO conversion during photocatalysis. Under lower energy irradiation (>500 nm) with added 3 vol% water in DMF solvent, the ZnP hybrid showed a TON_{Re} of ~2000 over an extended time-period of 50 h. It was found via in-situ UV-Vis absorption spectroscopy that the added porphyrin photosensitizers experience a significant photomodification during photolysis. Detailed in-situ mass analysis of supernatant after photocatalysis revealed that the original structure of porphyrin derivatives was significantly modified.

Poster Presentation : **INOR.P-88**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Visible-light-driven cleavage of the lignin β-O-4 bond using silver ion-exchanged zinc indium sulfide

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chemistry, Pukyong National University, Korea

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

Ternary metal chalcogenide, zinc indium sulfide (ZnxIn2Sx+3) is a typical visible-light-responsive photocatalyst which has a tunable band gap according to variable composition of Zn and Indium. Recently, ZnxIn2Sx+3 has been intensively utilized in photocatalytic valorization of lignin into functionalized aromatics. Herein, as facile strategy for promoting the photocatalytic activity of zinc–indium–sulfide (ZnxIn2Sx+3) for cleavage of the lignin β-O-4 bond under mild conditions, Ag+ exchange process was employed for tuning of the activity by modifying single atom catalytic site. Consequently, after Ag+ exchange, the photocatalytic yield of cleavage of the lignin β-O-4 enhanced up to ~50% compare to sample before ion exchange.

Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

The Effective Strategy of Encapsulating Metal-Sulfide Quantum Dot into Zeolitic Imidazolate Framework by Modification of QD with Identical Ligand

Yerim Son[*], **Hyun Sung Kim**[1,*]

Chemistry, Pukyong National University, Korea

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

The controllable encapsulation of metal-sulfide quantum dot into metal–organic has attracted significant research interest in a variety of fields. Typically, polyvinylpyridine(PVP) and mercaptopropionic acid(MPA) as capping materials are typically used to encapsulate QD into Zeolitic Imidazolate Framework. In our study, we have employed 2-mercaptoimidazole(MIm) as efficient capping materials for encapsulation into the Zeolitic Imidazolate framework(ZIF)-8. In particular, we have carried out the photocatalytic reaction with the prepared CdS QD(MIm)@ZIF-8 and others such as CdS QD@ZIF-8 composites using PVP and MPA. Only case of CdS QD(MIm)@ZIF-8, photocatalytic reduction of Methyl Viologen(MV^{2+}) was observed by quantum dots encapsulated in ZIF-8 crystals, but that bulky Diquat(DQ^{2+}) does not, which is consistent with efficient molecular sieving. The as-prepared CdS QD(MIm)@ZIF-8 composites exhibit functional photocatalytic properties that derive from the CdS QD molecular sieving that originate from the ZIF-8 framework.

Poster Presentation : **INOR.P-90**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Effective amine-functionalization of a MOF without solvent exchange

Doo San Choi, Yun Seok Chae, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Metal−organic frameworks (MOFs) have emerged as an extensive class of crystalline materials with ultrahigh porosity. Especially, amine-grafted Mg2(dobpdc) have been reported to show excellent CO2/N2 selectivities and adsorption characteristics. To synthesize amine-grafted Mg2(dobpdc), an immense amount of methanol is used. Methanol is a highly toxic liquid that may cause environmental issues. Herein, we optimized the best way to reduce methanol usage. These synthetic methods are confirmed by infrared spectroscopy, PXRD, SEM and gas sorption. Detailed synthetic scheme and specific properties will be presented in the poster.

Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Fabrication and CO2 adsorption properties of water-stable MOF-membrane

Yun Seok Chae, Doo San Choi, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Due to high surface areas, large porosity, tunable pore sizes, and functionalities, metal-organic frameworks(MOFs) have prospective application in field such as gas storage/separation. However, MOFs with advantageous features are readily degraded because the MOFs are collapsed upon exposure to water. We mixed a hydrophobic polymer with amine-functionalized MOFs to enhance water stability. The MOF-membrane was confirmed by PXRD, infrared spectroscopy. CO2 adsorption capacity was evaluated by thermogravimetric analysis (1000 ppm CO2 balanced with N2). Detailed synthesis and CO2 adsorption properties of the membrane will be presented in the poster.

Poster Presentation : **INOR.P-92**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Control of degree of photocatalytic lignin β-O-4 bond cleavage using silver ion-exchanged Zinc Cadmium Sulfide

SungGyu Lee, Hyun Sung Kim[1,*]

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

A series of ternary ZnxCd1-xS were prepared by a hydrothermal reaction as photocatalyst for lignin β-O-4 bond cleavage. The experimental results showed that the Zn0.25Cd0.75S photocatalysts exhibited a high photocatalytic activity for selectively cleave the rich C-O bond of the β-O-4 bond. Ag+ exchange process was employed into series of ternary ZnxCd1-xS for tuning of the activity by modifying single atom catalytic site. Here, we report that atomically dispersed Ag+ ion in wurtzite ZnxCd1-xS delivers an efficient and durable photocatalytic performance for highly substituted lignin model compound under visible range.

Poster Presentation : **INOR.P-93**
Inorganic Chemistry
Zoom 3 WED 16:30~17:00

Ortho-Donor-Appended Doubly Boron-doped TADF Emitters for Highly Efficient Green to Red OLEDs

Ajay Kumar, Hanif Mubarok, Kihoon Shin, Min Hyung Lee[*]

Department of Chemistry, University of Ulsan, Korea

Ortho-donor-appended doubly boron-doped thermally activated delayed fluorescence (TADF) emitters based on a 9,10-diboraanthracene (DBA) acceptor (Cz2oDBA, **2**; BuCz2oDBA, **3**; DMAC2oDBA, **4**) are prepared. X-ray diffraction analyses of **2** and **4** reveal the symmetrical and highly twisted *ortho*-donor□acceptor□donor (D□A□D) structure of the emitters. The twisted conformation leads to a very small singlet-triplet energy gap (□EST < 0.08 eV) that gives rise to strong TADF. The emission color is fine-tuned from green (**2**) to yellow (**3**) to red (**4**) depending on the strength of the donor moieties. Carbazole-containing **2** and **3** exhibit high photoluminescence quantum yields (PLQYs) approaching 100%, whereas DMAC-substituted **4** is moderately emissive (PLQY = 44%) in a doped host film. Highly efficient green-to-red TADF-OLEDs are realized with the proposed ortho-D□A□D compounds as emitters. The green and yellow OLEDs incorporating **2** and **3** as emitters exhibit high external quantum efficiencies (EQEs) of 26.6% and 21.6%, respectively. A red OLED fabricated with **4** exhibits a maximum EQE of 10.1% with an electroluminescence peak at 615 nm. The details of synthesis and photophysical and electroluminescent properties of the emitters will be discussed.

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Coordination cage compounds using a hexafluorosilicate anion; Competition between some polyatomic anions

Jeyeong Lee, Sangwoo Lim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

The self-assembly of $Cu(BF_4)_2 \cdot H_2O$ with 1,2-bis(dimethyl(pyridin-3-yl)silyl)ethane (L) at room temperature very slowly produce crystals consisting of the coordination cages, $[(SiF_6)@Cu_2L_4](BF_4)_2$. The reaction of CuX_2 ($X^- = BF_4^-$ and ClO_4^-) with L in the presence of $(NH_4)_2SiF_6$ fast gives rise to the cages $[(SiF_6)@Cu_2L_4](BF_4)_2$ and $[(SiF_6)@Cu_2L_4](SiF_6)$, respectively. Anion exchange of $[(SiF_6)@Cu_2L_4](BF_4)_2$ with NaX ($X^- = PF_6^-$ and NO_3^-) gives rises to a 2D structure of $[CuX_2L_2] \cdot H_2O$. The significant catalytic effects on catechol oxidation catalysis in dichloromethane have been observed in the order $[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH > [(SiF_6)@Cu_2L_4](SiF_6) \cdot > [Cu(PF_6)_2L_2] \cdot H_2O > Cu(BF_4)_2$.

Poster Presentation : **INOR.P-95**

Inorganic Chemistry

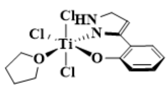
Zoom 3 WED 16:30~17:00

Titanium(IV) catalyst synthesis for Cycloaddition of CO_2 to epoxides by using ligand in various forms of nitrogen

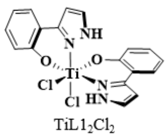
Junseong Lee*, Jung Seung hoo[1], Guitae Park[2], Jungwi Mok[2]

Department of Chemistry, Chonnam National University, Korea
[1]*chemistry, Chonnam National University , Korea*
[2]*chemistry, Chonnam National University, Korea*

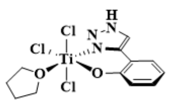
Global warming is rapidly intensifying in today's society due to CO_2 emissions from the atmosphere. In order to solve this problem, research is being actively carried out that can be used as a resource for living by using CO_2. Recent reports have shown that metal deposits have been used as catalysts to conduct chemical reactions of CO_2 and propylene oxide, resulting in the synthesis of propylene carbonate (PC), one of the useful products. PC is a highly utilized substance medical, photovoltaic film, monomer of polymer, electrolyte of secondary batteries. But the metals used in them, such as Co, Zn, and Al, are toxic and can cause environmental problems. Other literature suggests that titanium (Ti), which is often used as a catalyst, is also highly active in CO_2 reactions. Unlike other metals, titanium is a relatively safe and common metal, so it can be used environmentally and economically efficiently. We are trying to synthesize new titanium metal complexes using N-hetero cyclic ligand with different number and location of Nitrogen. These complexes were prepared by simple reaction of $TiCl_4$ and ligands and characterized by various analytical methods including NMR and HR-MS. Their molecular structures were also studied by X-ray crystallography. And using synthesized catalysts, we try to identify the expected activity through the reaction of CO_2 and propylene oxide.



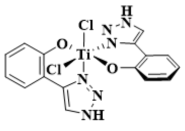
$TiL1_1Cl_3(THF)$



$TiL1_2Cl_2$



$TiL2_1Cl_3(THF)$



$TiL2_2Cl_2$

Poster Presentation : **INOR.P-96**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Directed synthesis of hollow gold-silver nanocatalysts for the active and efficient electroreduction of CO_2

Joon Woo Park, Hyunjoon Song*

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

Bimetallic nanocatalysts yield broader catalytic properties over monometallic catalysts, whereas controlling their properties to obtain the desired activity or selectivity is a major challenge in designing such materials. Especially in the field of CO_2 electroreduction, this approach has been widely applied with various metals including noble metals such as gold and silver.In this work, we report the application of gold-silver nanoparticles to the direct electrochemical reduction of CO_2. Through a simple galvanic replacement step, we obtained nanocubes with hollow structures which resulted in larger surfaces and catalytic currents for CO. Based on theoretical modeling of the nanoparticle surface, we validate the optimal point of the degree for galvanic replacement to obtain maximized surfaces along with moderate overpotentials. This endeavor shows prospects for economic nanocatalysts via alloying while retaining the catalytic performance of pure gold, and thus the importance of designing nanosurfaces in electrocatalysis.

Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Zoom 3 WED 16:30~17:00

Post-Synthetic Anion-Regulation toward Phosphosulfide Materials in Unique Hollow Toroidal Shape

Yongju Hong, Taekyung Kim, Jinhyoung Jo, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Post-modification of nanocrystals through cation exchange, creating composition-controlled nanostructure emerged, the feasible nanomaterials has been greatly diversified, but they are still limited in types of anion framework, of which the modulation is challenging due to the nature of sluggish diffusion kinetic. We introduce facile anion-modulation method using to create anion (P and S) hybridized copper phosphosulfide in the unique hollow toroidal morphology, based on Kirkendall effect and crystal structure relations. In this work, we revealed that the formation of hollow toroid shape is attributed to the in-situ formed vacancies and defects induced by desulfurization and migration of Cu^+ and provide a mechanism of shape and phase evolution. We expect that this anion-regulation method and the anion modulated-template can inspire the research of multi-anion structures and exploit new phosphosulfide materials.

Poster Presentation : **INOR.P-118**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Experimental and Theoretical Studies for the Zintl Thermoelectric $(Ca_{3-x}M_x)AlSb_3$ (M = Yb, Na, Nd) system

Yeongjin Hong, JunSu Lee, Tae-Soo You[*]

Department of Chemistry, 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. Zintl phase can be considered as an intermetallic compound composed of electropositive alkali and alkaline-earth metals elements and electronegative main-group metals or semimetal. Zintl phase compounds are valuable for thermoelectric applications at high temperatures. 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 $AlSb_4$ tetrahedra. The novel Zintl phase series $Ca_{3-x}M_xAlSb_3$ (M = Na, Nd, Yb; 0≤x≤0.4(2)) is consist of five compound as Ca_3AlSb_3 (loaded composition $Ca_5Al_2Sb_{5.3}Sn_{0.7}$, $Ca_3AlSb_{2.7}Ge_{0.3}$), $Ca_{2.97(1)}Nd_{0.03}AlSb_3$, $Ca_{2.59(2)}Yb_{0.41}AlSb_3$, $Ca_{2.95(3)}Na_{0.05}AlSb_3$. These compounds were synthesized by the arc-melting method, and their crystal structures were characterized by both powder and single-crystal X-ray diffractions. Dopants including Na, Nd, Yb, Ge in the $Ca_{3-x}M_xAlSb_3$ system is Ca-rich compound. Quite interestingly, $Ca_{3-x}M_xAlSb_3$ 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. However, the p-type dopant of Ge was not included. 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. In particular, as Ca and Yb are mixed, the DOS level was relatively lower at the Fermi level, and this region was slightly wider than the other compounds. In the case of Nd and Na doped compounds, the Fermi level was shifted due to the influence of electrons. The chemical composition analyzed by EDS indicated $Ca_{2.59(2)}Yb_{0.41}AlSb_3$, which was quite close to the SXRD result.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Two Steps to Improve the Thermoelectric Performance of the Ca$_{5-x}$Yb$_x$Al$_{2-y}$In$_y$Sb$_6$ System

Junsu Lee, Tae-Soo You*

Department of Chemistry, Chungbuk Natioanl University, Korea

Previously, our research group reported the thermoelectric (TE) Zintl phase Ca$_{5-x}$Yb$_x$Al$_2$Sb$_6$ ($1.0 \leq x \leq 5.0$) system, synthesized Yb-rich compounds underwent the structural transformation from the Ba$_5$Al$_2$Bi$_6$-type to the Ca$_5$Ga$_2$Sb$_6$-type phase via the post-heat treatment. To enhance the TE properties of this system, we attempted the Al substitution for In resulting in producing the Ca$_{5-x}$Yb$_x$Al$_{2-y}$In$_y$Sb$_6$ ($3.07(1) \leq x \leq 4.88(2)$; $y = 0.16(2), 0.32(1), 2.00$) solid-solution system. The title compounds were successfully synthesized by arc-melting and characterized by both powder and single-crystal X-ray diffractions. The initially synthesized Yb-rich compound also underwent the structural transformation from the Ba$_5$Al$_2$Bi$_6$-type to Ca$_5$Ga$_2$Sb$_6$-type phase via the post-heat treatment at 973 K for 1 month. Both of two title structures of the Ba$_5$Al$_2$Bi$_6$-type and Ca$_5$Ga$_2$Sb$_6$-type phases adopt the orthorhombic space group Pbam ($Z = 2$, $oP26$) with total seven independent atomic sites including three Ca sites, three Sb sites, and one Al sites in a unit cell. Interestingly, Al/In mixed compound showed increased electrical conductivities than only Al compound, and it was due to the lighter carrier effective mass of In than Al. As a result, the *ZT* of Ca$_{1.14(2)}$Yb$_{3.86}$Al$_{1.68(1)}$In$_{0.32}$Sb$_6$ (Ca$_5$Ga$_2$Sb$_6$-type) has increased about 4 times in comparison to its quaternary predecessor Ca$_{1.55(1)}$Yb$_{3.45}$Al$_2$Sb$_6$ (Ca$_5$Ga$_2$Sb$_6$-type). In addition, a series of theoretical calculations using tight-binding linear muffin-tin orbital (TB-LMTO) method also provided understanding about the chemical bonding and electronic structures of title compounds based on DOS and COHP analyses, and compared the electronic energy difference between the Ca$_5$Ga$_2$Sb$_6$-type and the Ba$_5$Al$_2$Bi$_6$-type phase for the given Yb-rich composition

Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Influence of the *p*-type Double Dopants for the Thermoelectric Properties of Zintl Phase and Crystal Growth of $Ca_{11-x}A_xSb_{10-y}Ge_z$, $(0 \leq x \leq 9; 0 \leq y \leq 3; 0 \leq z \leq 3)$

Hayeon Sa, **Tae-Soo You**[1,*]

Department of chesmitry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

We recently reported the effects of multi-substitution for the thermoelectric (TE) performance in the $Ca_{11-x}Yb_xSb_{10-y}Ge_z$ $(0 \leq x \leq 9; 0 \leq y \leq 3; 0 \leq z \leq 3)$ system. In that study, we exploited the two-track strategy using two different *p*-type substitutions: (1) the cationic Yb mixing for Ca and (2) the anionic Ge doping for Sb, and the influence of these multi-substitutions for electronic structures as well as TE performance were thoroughly studied. In order to further expand this series of multi-substituted *p*-type Zintl TE materials, we investigated the double *p*-type doping using both the cation and anion sites in the $Ca_{11-x}A_xSb_{10-y}Ge_z$, (A = Na, Li; $0.06(3) \leq x \leq 0.17(5)$; $0.19(1) \leq y \leq 0.72(1)$, $0.22(1) \leq z \leq 0.45(1)$) system. In this work, we respectively introduced two different monovalent cations, Li and Na, along with the anionic Ge dopant. Two title compounds in the $Ca_{11-x}A_xSb_{10-y}Ge_z$ system have been synthesized by arc-melting and lead flux synthesis, and characterized by both powder and single crystal X-ray diffractions. They crystallized in the isotypic $Ho_{11}Ge_{10}$-type structure (tetragonal space group *I*4/*mmm*, Pearson symbol *tI*84) with nine crystallographically independent atomic positions in each unit cell, which include one Ca^{2+}/A^{+} mixed-cationic site and one Sb/Ge mixed-anion site. The overall crystal structure can be described as an assembly of three different types of co-facial polyhedra formed by Ca^{2+}/A^{+}, which of each is centered by isolated Sb atoms. The 3-D anionic framework can be considered as an assembly of the dumbbell-and square-shaped Sb atoms. The $Ca_{11-x}A_xSb_{10-y}Ge_z$ has high crystallinity, forming visible crystals even under the facile arc-melting method. Fully grown octahedral crystals were formed under lead flux synthesis. To further investigate the overall electronic structure and chemical bonding in the title compounds, a series of DFT calculations using TB-LMTO-ASA method were performed for two hypothetical structural models of $Ca_{10.5}A_{0.5}Sb_{9.5}Ge_{0.5}$ (A = Li, Na). In addition, DOS, COHP, ELF and band structures were also calculated.

1. G. Nam; W. Choi; J. Lee; S. Lim; H. Jo; K. Ok; K Ahn and T.-S. You, Inorg. Chem, 2017, 56, 7099-

7110.2. J. Lee; K. Ahn; K. Kim; H. Jo; J. Yoon; D. Moon; W. Shin; K. Ok and T.-S You, Cryst. Growth Des, 2019, 19, 3498-3508.3. J. Lee; H. Sa; H. Jo; D. Moon; K. Ok and T.-S You. Cryst. Growth Des. 2020, 20, 4503-4511.

Poster Presentation : **INOR.P-121**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Noble Metal Nanoparticle@Hollow Mesoporous Carbon with FeCo/Graphitic Shell Nanoparticls as Magnetically Recyclable Yolk–Shell Nanocatalysts

Eunseo Hong, Won Seok Seo*

Department of Chemistry, Sogang University, Korea

We have developed highly stable and magnetically recyclable yolk–shell nanocatalysts for catalytic reduction of nitroaromatics. These nanocatalysts are composed of a catalytic metal nanoparticle encapsulated in a hollow mesoporous carbon (hmC) shell with a thickness of ~15 nm. The hmC shell contains ~6 nm FeCo/graphitic carbon shell (FeCo/GC) nanoparticles. We have synthesized the catalytic metal@hmC-FeCo/GC nanocatalysts by thermal decomposition of Fe and Co precursors in silica of a solid core/mesoporous shell structure containing a catalytic metal nanoparticle within the core, subsequent ethylene chemical vapor deposition (CVD), and then removal of the silica by treatment with aqueous HF. The catalytic metal@hmC-FeCo/GC has superparamagnetism and high saturation magnetization at room temperature. It also shows a type IV sorption isotherm, typical for mesoporous carbon (pore diameter = ~4 nm), thereby ensuring ready accessibility to the catalytic metal core by substrates. We have shown that the catalytic metal@hmC-FeCo/GC catalyses the reduction of 4-nitrophenol and 4-nitrotoluene more efficiently than the catalytic metal nanoparticles do, can be separated very quickly from the reaction mixture using a magnet, and can be reused for the same reduction reaction at least five times without loss of the initial level of catalytic activity.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Mesoporous Silica Nanospheres Embedded with FeCo/Graphitic Shell Nanoparticles as Magnetically Recyclable Adsorbents

Eunseo Hong, Won Seok Seo*

Department of Chemistry, Sogang University, Korea

Highly stable and magnetically separable mesoporous silica nanospheres (MSNs) embedded with 4.6±0.8nm FeCo/graphitic carbon shell nanocrystals (FeCo/GC NCs@MSNs) were synthesized by thermal decomposition of metal precursors in MSNs and subsequent methane CVD (chemical vapor deposition). The FeCo/GC NCs@MSNs had a high specific surface area (442 m^2 g^{-1}), large pore volume (0.65 cm^3 g^{-1}), and tunable size (65 nm, 130 nm, and 270 nm). Despite the low magnetic metal content (8.35 wt%), the FeCo/GC NCs@MSNs had a sufficiently high saturation magnetization (17.1 emu g^{-1}). This is due to the superior magnetic properties of the FeCo/GC NCs, which also enable fast magnetic separation of the nanospheres. The graphitic carbon shell on the FeCo NCs not only protects the alloy core against oxidation and acid etching in 35% HCl(*aq*), but also facilitates non-covalent, hydrophobic interactions with the hydrocarbon chains of organic dyes such as methyl orange and methylene blue. Surface functionalization of the FeCo/GC NCs@MSNs with thiol groups provides efficient capacity for binding with Hg^{2+} ions. We have shown that the thiol-functionalized FeCo/GC NCs@MSNs (FeCo/GC NCs@MSNs-SH) work as multifunctional adsorbents for organic dyes (target organic pollutants) and Hg^{2+} ions (target inorganic pollutant). We also demonstrated that the FeCo/GC NCs@MSNs-SH are excellent recyclable adsorbents for methyl orange.

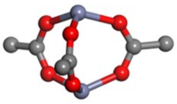
Poster Presentation : **INOR.P-123**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Compilation of Kinetic and Thermodynamic Structures of Zn-based Metal-Organic Frameworks

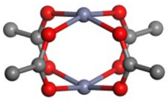
Junsu Ha, Jaehwa Lee, Jaehui Kim[1], Hoi Ri Moon[*]

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

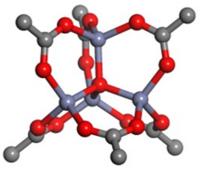
Metal-organic frameworks (MOFs) are highly ordered porous materials constructed by coordination bonds between inorganic and organic species. Because the intrinsic properties of each framework are attributed to their structure, many researchers made the intensive efforts to extend structural diversity of MOFs and construct the desired structures. Reticular chemistry enables the prediction of the underlying topology of MOFs, which consist of a diverse combination of secondary building units (SBUs) and multi-topic linkers. However, in an actual synthetic environment, even the same pair of metal ion and linker results in totally different SBUs by structural complexities caused by a simple change in synthetic condition. For this reason, several studies try to demonstrate the relationship between this structural diversity and synthetic nature. The structure control has been widely studied to describe this issue, but most of the studies only focused on the effect of a single factor or provided a lack of the relationship between each synthetic parameter. Herein, we present the effect of synthetic temperature, metal/ligand ratio and solvent to control the kinetic or thermodynamic frameworks and the relationship between each synthetic parameters. The entire works were demonstrated by the selective crystallization of five different MOFs having different SBUs (Zn_4O, 3, 4-paddle-wheel, Zn_6), from one of the most well-known Zn_4O SBU to thermodynamically unfavored 3-paddle-wheel SBU, and connectivity (3, 4, 6, 7, 10-points of extension) by systematically controlled syntheses using Zn(II) and 1,4-naphthalenedicarboxylic acid.



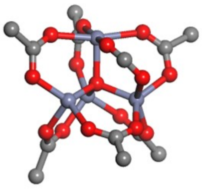
$Zn_2(COO)_3$
3-connected



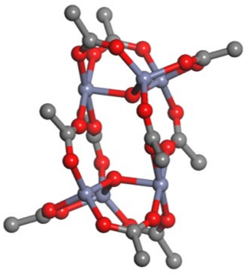
$Zn_2(COO)_4$
4-connected



$Zn_4O(COO)_6$
6-connected



$Zn_4O(COO)_7$
7-connected



$Zn_6(OH)_2(COO)_{10}$
10-connected

Poster Presentation : **INOR.P-124**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Synthesis of Heterometallic Supramolecular Assembly with Pyridyl functionalized β-Diketonate Metalloligands

Neetu Singh, **Junseong Lee**[1,*]

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We report the synthesis of novel heterometallic supramolecular assemblies with Pt and Pd fragments using cyclometallated Ir(III) metalloligand containing pyridyl functionalized β-diketonate ligand, as a building block. The Ir-metalloligand building block and their assemblies were characterized by multinuclear (^{1}H and (^{31}P) NMR, DOSY NMR, IR, EA, ESI-MS and single crystal X-ray diffraction. The design and synthesis of pyridyl functionalized β-diketonate based metalloligand are attractive for use in self-assembly of mixed-metal supramolecular architectures, which can further utilizes for several applications such as, encapsulation of guest molecules, catalysis, optoelectronic, drug-delivery and bioimaging. The chelating nature of bidentate O, O donor are relative low lability, while the negative charge on the ligand allows to form a neutral metal complexes. Therefore, pyridyl functionalized β-diketonato ligands, apart from acting as a chelating agent to the primary metal center, can donate the attached pyridyl groups to secondary metals to generate a designed supramolecular architectures.

Poster Presentation : **INOR.P-125**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Mechanism study of directed C-H arylation using heterogeneous aryl-Pd(II)-oxo clusters

Minjun Kim, Hyunjoon Song[*]

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

Hetero-aromatic compounds such as indole and benzofuran, which are used as building blocks for drug or natural products, have been widely studied. The traditional way of C-H arylation was to use C-C coupling reactions, but recently, diaryliodonium oxidants have been used to selective C-H arylation. Particularly, Glorius and co-workers reported heterogeneous C-H arylation using Pd/C and diaryliodonium salts and proposed mechanistic studies proceeding via a Pd(0)/Pd(II) systems by kinetic studies. However, the accurate structure of active species have not yet been identified. In this presentation, we report the active species for heterogeneous C-H arylation of hetero-aromatic compounds via diaryliodonium salts. Well-defined Pd NPs have been used to precise analysis for active species of which coordination chemistry has been determined using X-ray absorption fine structure (XAFS).

Poster Presentation : **INOR.P-126**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Interaction studies between ConA and N-linked glycans

Seung Jae Lee*, **Yung Min Lee**

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

The binding abilities of lectins brought attentions due to the specific interactions with carbohydrates and they are applied to diverse fields of biotechnologies including detection, isolation, and concentration of biological molecules. Among these lectins, biochemical aspects of concanavalin A (ConA) has intensively studied trough structural and functional investigations. The X-ray crystallography proved that ConA has two β-sheets and a short α-helix as a form of metalloprotein that housed with Mn^{2+} and Ca^{2+}. These heterometals were coordinated with side chains Asp, Glu, His, and Asn residues and it finally affects the structural environments through hydrogen bonds to hydroxyl moieties in carbohydrates. Recent studies proved that ConA can regulate biophysical interactions to pathogens such as viruses through glycoproteins in enveloped viruses. ConA generates specific interactions with diverse polysaccharides through Tyr, Asn, Asp, and Arg residues positioned next to metal coordinated region. The generation of self-assembled complex reported that ConA can form diverse complex including monomer, dimer, trimer, and tetramers. Further applications of ConA can cause unstable results due to these diversities. In this presentation, the structural modification through replacements of metal ions and formation of complexes in ConA will be described. The substitution of metal-coordinated region through transition metal ions causes conformational shifts in carbohydrate binding regions and this affects complex formation. These events indicates that lectins need to be thoroughly investigated based on their biophysical media to avoid unexpected changes.

Poster Presentation : **INOR.P-127**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

C–H and O_2 activation through component interactions based on the ratio of substrates in hydroxylase

Seung Jae Lee*, Yunha Hwang, Dong-Heon Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

The specific enzymatic activities of sMMO are widely investigated to understand its enzymatic activity and turnover rate to understand the influence by substrates including hydrocarbons, molecular oxygen, electrons, and proton. The ratio between substrates and enzymes need to be further investigated to understand its possible influences during expression of hydroxylase and other auxiliary enzymes. In this presentation, the expression of MMOH is described based on the ratio of two substrates including methane and oxygen. The expression level in sMMO is important for the purification of this homodimer ($\alpha_2\beta_2\gamma_2$) and the complex formation of six subunits needs to discover further mechanism studies through MMOG. The methane oxidation is performed in α-subunit of MMOH and β-subunit generates specific interactions for the dimeric formation of hydroxylase component. The function of γ-subunit is not well quite understood, but this small-subunit only detected in water-soluble region after cell-lysis. The methane concentration of sMMO proved that the injection volume of methane and molecular oxygen (O_2) affect the volume of soluble portion of MMOH based on the quantitative analysis. In addition, the differences of these species depend on the concentration of γ-subunit. The specific enzyme activities are also affected by the concentration of methane and oxygen in buffer. The catalytic activities of enzymes are influenced by the ratio of reductase components and high concentration of oxygen decrease the activities.

Poster Presentation : **INOR.P-128**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Electron transfer and its functional effects by MMOR in FAD binding domain from *M. sporium* 5

Seung Jae Lee*, Chungwoon Yoon, Dong-Heon Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

The resting state of MMOH is reduced by the addition of electrons through MMOR and reduced di-iron active site (Fe^{II}-Fe^{II}) can activate molecular oxygen (O_2) for C–H activation. The essential intermediates from P*, H_{peroxo}, and Q can be generated by the O_2 activation from reduced MMOR, but the accurate electron-transfer pathways need to be further elucidated. MMOR has two cofactors including FAD/NADH-binding domain (MMOR-FAD) and [2Fe-2S] cluster to transfer electrons from NADH to di-iron active site housed in α-subunit MMOH. Although the structural information is available from solution nuclear magnetic resonance (NMR) of each domain, MMOR-FAD and MMOR-Fd, due to the size of molecule (39-kDa), the overall structure needs to be further discovered.The reductase component from *Methylosinus sporium* 5 is successfully expressed and purified to understand biophysical aspects. The FAD content and ferrozine assay confirmed that presence of these cofactors and UV-vis spectra proved the presence of FAD (394 and 485 nm) and [2Fe-2S] cluster (332, 418, and 467 nm). The crystallization of MMOR provides structural insight of truncated version of MMOR-FAD binding domain generated by protease activity. The residues including S159, S160, Y161, and S184 generated hydrogen bonds with FAD with 2.5 – 3.5 Å apart. The mutated MMOR was successfully purified and confirmed the modification of iron contents and concentration of FAD. These results confirmed that the expression of reductase components affects the cofactor interactions of MMOR. In addition, the modification of MMOR-FAD affects the structural components of iron-sulfur clusters.

Poster Presentation : **INOR.P-129**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Mutational studies of MMOR and their influences of binding affinity to hydroxylase in reduced and oxidized states

Seung Jae Lee[*], **Chae Min Lee**

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

Methane (CH_4) is considered as one of the most important greenhouse gases owing to its 20-fold higher heat capacity compared with that of carbon dioxide (CO_2). Preliminary studies have aimed to elucidate the mechanisms of soluble methane monooxygenase (sMMO) involved in this extremely stable C–H activation (104.9 kcal/mol) through intermediate studies, advanced spectroscopies, and structural researches, mostly in *Methylosinus trichosporium* OB3b and *Methylococcus capsulatus* Bath, although mechanistic studies are still required. In this study, *M. sporium* 5 was cultured in a tightly regulated NMS media by supplying methane and air to understand its growth and the expression levels of multi-component enzymes. MMOH was found to be highly expressed in *M. sporium* 5, and it was purified to evaluate its catalytic activities using diverse substrates. MMOB and MMOR were also expressed in *E. coli* via constructed plasmids to obtain highly purified enzymes. The successfully expressed and purified enzymes were utilized to measure specific enzyme activities (SEA), and these results showed that *M. sporium* 5 exhibits optimal activity at pH 7.5. The electron transfer environment of MMOR is crucial for the activity of sMMO, and different acidities may change the electron transfer environment. In vitro activity measurements demonstrated that alkanes, halogens, benzene, and toluene are oxidized through sMMO, and 2 mol equivalents of MMOB showed optimal activity.

Poster Presentation : **INOR.P-130**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Influence of chaperone protein, MMOG, to hydroxylase for the conformational changes to MMOH

Seung Jae Lee*, Chae Min Lee, Ka Young Son, Dong-Heon Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

The catalytic activities of soluble methane monooxygenases (sMMO) are regulated by the interactions of between hydroxylase and other auxiliary enzymes including regulatory components and reductase. The physical map of sMMO genes has confirmed that *mmoG* gene positioned 5'- or 3'-region in sMMO and the expressed sequence of amino acids show high sequence homologies with reported chaperone. This chaperone, MMOG, is successfully expressed to understand its functions in sMMO system from synthesized gene from *Methylosinus sporium* 5, a type II methanotroph. The expressed enzyme is purified with anion exchange and size-exclusion column more than 95% purity and its biophysical aspects were investigated. The UV-vis spectroscopic studies proved that MMOG does not interact with NADH when it purified with two-step process. The binding affinity is measured through the fluorescence measurements through tryptophan quenching. This results indicate that The 1:1 binding model fitting demonstrated competitive binding affinity to other auxiliary enzymes which implies that MMOG will share the binding site, di-iron active site, like regulatory or inhibitory enzymes and reductases. The functional consequence of MMOG is important to elucidate its physiological functions and catalytic activities are investigated whether it accelerates or retards specific enzyme activity. In this presentation, the biophysical aspect of MMOG will be discussed to understand functional and structural roles in sMMO system.

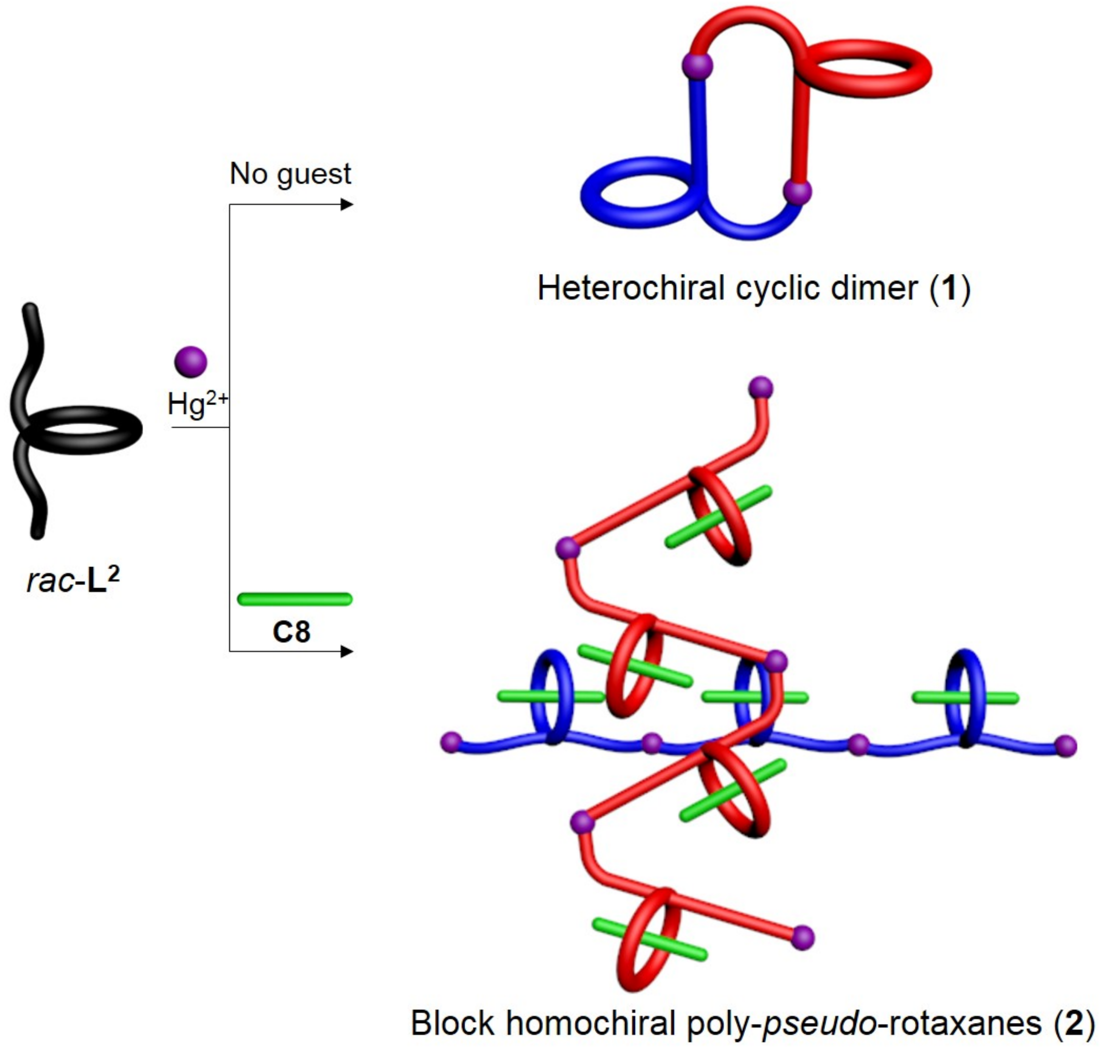
Poster Presentation : **INOR.P-131**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Coordinative Linking of rac-A1/A2-Difunctionalized Pillar[5]arene: Heterochiral Cyclic Dimer and Homochiral Poly-pseudo-rotaxanes

Seulgi Kim, **Eunji Lee**[1], **In-Hyeok Park**[2], **Shim Sung Lee**[*]

Department of Chemistry, Gyeongsang National University, Korea
[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*
[2]*Graduate School of Analytical Science and Technology, Chungnam National University, Korea*

The influence of organic guests on the supramolecular coordinative linking of di-functionalized pillar[5]arene is reported. Reaction of a racemic A1/A2 di-thiopyridyl pillar[5]arene (*rac*-**L**) with mercury(II) chloride afforded a heterochiral cyclic dimer complex $[\mathrm{Hg_2}(p\mathit{S}\text{-}\mathbf{L})(p\mathit{R}\text{-}\mathbf{L})\mathrm{Cl_4}]\cdot 2\mathrm{CH_2Cl_2}$ (**1**) in which the two mercury(II) atoms and a (*pS*-**L**)/(*pR*-**L**) pair come together to make a [2+2] metallacycle. Same reaction in the presence of the dinitrile guest **C8**, $[\mathrm{CN(CH_2)_8CN}]$, yielded a one-dimensional poly-pseudo-rotaxane $\{[\mathrm{Hg}(\mathbf{C8}@p\mathit{S}\text{-}\mathbf{L})\mathrm{Cl_2}][\mathrm{Hg}(\mathbf{C8}@p\mathit{R}\text{-}\mathbf{L})\mathrm{Cl_2}]\cdot 3\mathrm{CH_2Cl_2}\}_n$ (**2**). In **2**, *pS*-**L** and *pR*-**L** form two separated linear and zigzag types of homochiral poly-pseudo-rotaxanes in a crystal, respectively, both in parallel arrangement on each layer and the alternated layers stack perpendicularly adopting a firewood stacking motif. A pathway for the formation of the cyclic dimer complex and the poly-pseudo-rotaxane through the cyclic dimer is proposed.


No guest
Hg2+
rac-L2
C8
Heterochiral cyclic dimer (1)
Block homochiral poly-pseudo-rotaxanes (2)

Poster Presentation : **INOR.P-132**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

1,2-Dicarbonyl Radicals with Remarkable Physiological and Chemical Stability

Youngsuk Kim, **Eunsung Lee**[*]

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

Air- and water-stable organic radicals have great potential as spin labels or contrast agents for bio-imaging application. For example, there is extensive interest in the development of gadolinium-free organic radical contrast agents for magnetic resonance imaging (MRI). However, majority of organic radicals are unstable or insoluble in biological conditions, which continues to limit their application. Up to date, sterically hindered aminoxyl radicals show significant potential due to their accessibility and functionalizability. Although aminoxyl radicals show reasonable stability toward water, they rapidly decompose to hydroxylamines under physiological conditions without steric protection, due to reducing agents such as ascorbate. Here we designed and synthesized a new small molecule organic radical based on 1,2-dicarbonyl scaffold. The presented radicals showed superior stability towards physiological conditions (half-life of ~3000 hours) and are resistant towards chemically reducing, oxidizing, acidic, basic conditions, and high temperature. This remarkably stable radical will be a good platform for developing biologically stable organic radicals for bio-imaging application.

Poster Presentation : **INOR.P-133**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Hexagonal Tungsten Oxides with Very Large Bandgaps Designed by a Chemical Substitution-Oriented Method

<u>Geonju Park</u>, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

New hexagonal tungsten oxide materials designed by a chemical substitution-oriented method have been successfully synthesized via hydrothermal reactions. Despite the stoichiometric equivalence, the reported materials crystallize in the centrosymmetric space group, $R\text{-}3m$ and noncentrosymmetric space group, $P6_3mc$, respectively, depending on their counter cations. UV-vis diffuse reflectance spectroscopic analysis indicates that one of the reported materials exhibits the largest bandgap among all known phase-matchable nonlinear optical selenite compounds. Powder second-harmonic generation (SHG) measurements indicate the reported material reveals an SHG efficiency of *ca.* 1.1 times that of KDP and is type-I phase-matchable. A complete spectroscopic and thermal characterizations, calculations, and factors influencing the macroscopic centricity will be presented.

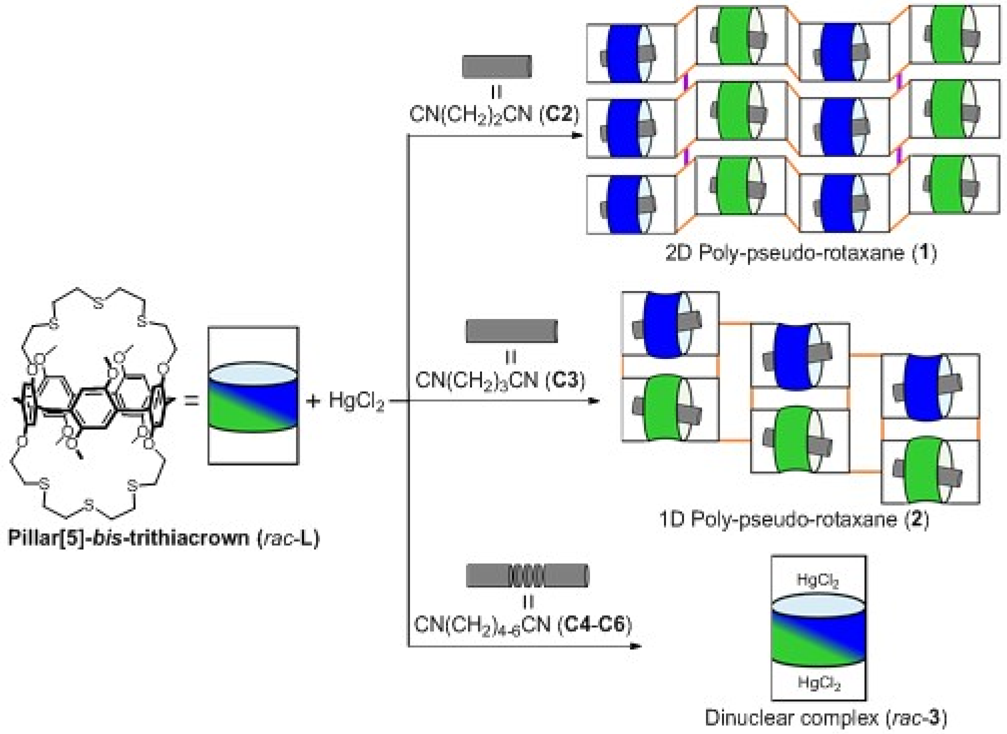
Poster Presentation : **INOR.P-134**
Inorganic Chemistry
Zoom 3 WED 17:00~17:30

Influence of Host-Guest Interactions on the Coordination Networking of Pillar[5]-bis-trithiacrown: 1D and 2D Poly-pseudo-rotaxanes

Mingyeong Shin, In-Hyeok Park[1], Eunji Lee[2], Shim Sung Lee[*]

Department of Chemistry, Gyeongsang National University, Korea
[1]*Graduate School of Analytical Science and Technology, Chungnam National University, Korea*
[2]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Pillar[5]-*bis*-trithiacrown (**L**) was employed as a ditopic host both for metal ion and organic guest. Herein we report the influence of dinitrile guests [$CN(CH_2)_nCN$ (n = 2-6: shortly **C2**-**C6**)] on the coordination networking of **L**. Assembly reaction of **L** with $HgCl_2$ in the presence of the **C2** guest afforded a two-dimensional (2D) coordination polymer **1**, $[Hg_3Cl_6(\mathbf{C2@L})]_n$ in which the **C2** guest occupies the cavity to give a (**C2@L**) unit and linking of these units by Hg-Cl-Hg bridges generates one-dimensional (1D) chains which are further crosslinked by Hg-$(\mu\text{-Cl})_2$-Hg units, giving rise the 2D rectangular grid. When the above synthetic procedure was repeated with the **C3** guest, a 1D coordination polymer **2**, $[Hg_3Cl_6(\mathbf{C3@L})]_n$ was isolated. In **2**, the **C3** guest occupies the cavity and two (**C3@L**) units and two Hg-Cl-Hg bridges form a cyclic dimer, resulting in the generation of a poly(cyclic dimer) via other two Hg-Cl-Hg linkages. The use of the longer guests **C4**-**C6** in the same reactions, however, yielded a discrete dimercury(II) complex **3**, $[Hg_2Cl_4(CH_3CN@\mathbf{L})]$, instead of coordination networks due to the unfavorable longer lengths of the guests. The observed results show that the formation of coordination networks and their morphologies are sensitive not only to the inclusion of dinitrile guests but also to the lengths of the dinitriles included due to the confined interior space of **L**, suggesting the organic guests as a potent controlling factor.


Pillar[5]-bis-trithiacrown (rac-L)
=
+ $HgCl_2$
II
$CN(CH_2)_2CN$ (C2)
2D Poly-pseudo-rotaxane (1)
II
$CN(CH_2)_3CN$ (C3)
1D Poly-pseudo-rotaxane (2)
II
$CN(CH_2)_{4-6}CN$ (C4-C6)
$HgCl_2$
$HgCl_2$
Dinuclear complex (rac-3)

Poster Presentation : **INOR.P-135**

Inorganic Chemistry

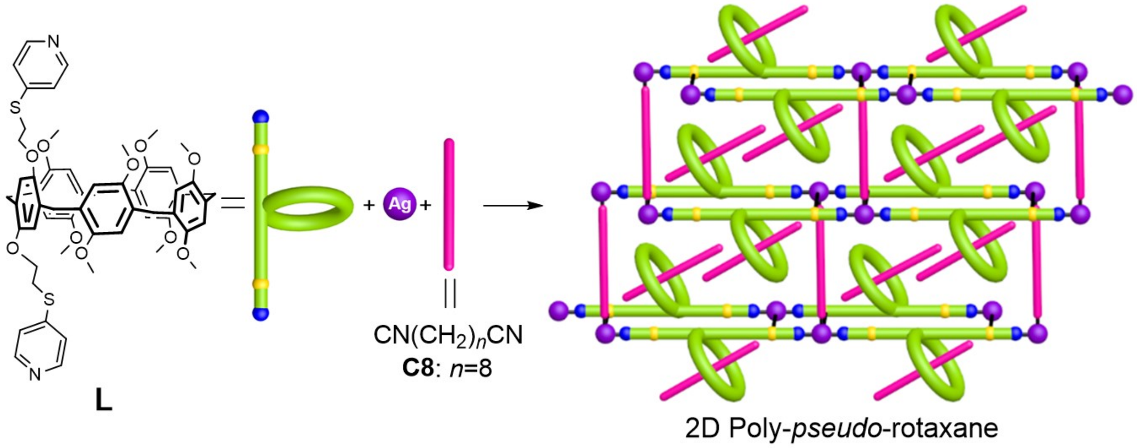
Zoom 3 WED 17:00~17:30

Formation of a Pillar[5]arene-Based Two-Dimensional Poly-Pseudo-Rotaxane where the Same Guest “Threads and Crosslinks”

Eunji Lee, Yoichi Habata[1], Shim Sung Lee[2,*]

Department of Chemistry, Gangneung-Wonju National University, Korea
[1]Department of Chemistry, Toho University, Japan
[2]Department of Chemistry, Gyeongsang National University, Korea

Reaction of thiopyridyl-armed pillar[5]arene (**L**) with $AgCF_3CO_2$ in the presence of the linear dinitrile guest molecule **C8**, [$NC(CH_2)_nCN$, n = 8], afforded a two-dimensional (2D) poly-pseudo-rotaxane $\{[(\mu_4\text{-}Ag)_2(\mathbf{C8@L})_2(\mu\text{-}\mathbf{C8})](CF_3CO_2)_2\}_n$. Interestingly, the guest molecule **C8** act as not only threads into the pillar[5]arene cavity but also crosslinks the 1D coordinative polymeric chains. The formation of the 2D poly-pseudo-rotaxane is driven by an adaptive rearrangement of the components that minimize the steric hindrance “between the threaded and crosslinked guests” well as “between the threaded guests”. A pathway for the formation of the 2D poly-pseudo-rotaxane is proposed.



Poster Presentation : **INOR.P-136**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Nanoscale-confined shape transformation of gold nanorods inside ZIF-8

Cheongwon Bae, Juyeong Kim[*]

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 52828, Korea

Hybrid nanostructures, composed of metal nanoparticle cores and porous inorganic shells, have shown new functions and properties. Various combinations between core and shell materials have been attempted for desired applications, which inevitably require much effort and time in material-dependent synthesis development. We demonstrate template-confined chemical transformation of a gold nanorod core encapsulated by a zeolitic imidazolate framework (ZIF) through oxidative etching and reductive regrowth while maintaining the ZIF shell structure. We discover template-dependent behavior of the nanorod core during its morphological transformation inside ZIF, displaying sluggish etching of the nanorod core and its shell-directed overgrowth. Our mechanistic understanding is supported by quantitative analysis on the core geometry and curvature as well as comprehensive control experiments. This will aid in the facile design of core-shell hybrid nanomaterials and advanced understanding in nanoscale-confined reactions.

Poster Presentation : **INOR.P-137**

Inorganic Chemistry

Zoom 3 WED 17:00~17:30

Lewis-Base Characteristics of Chloroform and Its Coordination Ability at Metal Center of Paddlewheel Metal-Organic Framework

Sun Ho Park, Nak Cheon Jeong[1,*]

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[1]*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Metal-organic frameworks (MOFs) have shown their critical potentials as crystalline porous solid materials in contemporary chemistry. In particular, MOFs with open coordination sites (OCSs), where Lewis-basic guest molecules can be coordinated excessively at their axial position, often function vital roles in potential applications such as catalysis, gas absorption, gas separation, drug delivery, chemical sensing, electronics, and ionic conduction. Thus, the chemical function of OCS has been considered as a quite important factor in such applications. Nevertheless, the coordination nature of the OCS still remains as a challenging issue. In this presentation, we show the coordination ability and Lewis-basic nature of chlorine atom in chloroform that has been commonly known as a non-coordinating molecule. For examples, we have observed the possible coordination of the chloroform via monitoring real-time in situ NMR and ex situ Raman spectra. On the basis of the observation, therefore, we propose not only the coordination ability of chloroform but also "coordination equilibrium" that is formed via the coordination exchange of strong Lewis-basic molecules (e.g., H_2O, MeOH, EtOH, and DMF) with weak Lewis-basic molecules, chloroform.

Poster Presentation : **INOR.P-158**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Enhancement of Efficiency of InP/ZnSeS/ZnS Quantum Dots using Bidentate Ligands

Hyeongjin Lee, Sang Wook Park[1], Young rag Do[2,*]

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[1]*Ddepartment of Chemistry, Kookmin University, Korea*
[2]*Department of Bionano Chemistry, Kookmin University, Korea*

Quantum dots (QDs) are promising materials for lighting applications because of their high photo luminescent quantum yields (PLQYs) and narrow full-width at half-maximum (FWHM). However, Cd-based and all-inorganic perovskite QDs involve heavy metals, such as Cd and Pb, which are prohibited by RoHS regulations. Meanwhile, InP/ZnSeS/ZnS QDs are heavy-metal free, and they do not violate RoHS regulations. For this reason, InP/ZnSeS/ZnS QDs have an advantage in the display market. In order to use InP/ZnSeS/ZnS QDs as display products, the higher the efficiency and stability, the better. However, ligand detachment by air, thermal damage, and UV of the InP/ZnSeS/ZnS QDs can cause a decrease in efficiency. Therefore, we improved the efficiency by causing the ligand to be more strongly bound by using a bidentate ligand such as 2,2-iminodibenzoic acid (IDA). The PLQY of IDA-treated InP/ZnSeS/ZnS QD is 25.5% higher than that of pristine sample.

Poster Presentation : **INOR.P-159**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Patterned electric field induced poly(ε-caprolactone) nanofiber alignment using electrospinning

Cheolbae Lee, Yoobeen Lee[1], Jin Seok Lee[1,*]

Department of chemistry, Hanyang University, Korea
[1]*Department of Chemistry, Hanyang University, Korea*

Research on nanofiber alignment has already been done a lot. But it still doesn't completely control the orientation of the fiber. We report the fabrication of scaffolds consisting of aligned poly(ε-caprolactone) nanofibers by utilizing a collector composed of a central hole and a patterned peripheral holes on metal substrate. This novel class of scaffolds was able to present nanoscale topographic cues to cultured cells, directing and enhancing their migration to aligned nanofiber. We also demonstrated that such scaffolds could induce faster cellular migration and population than random nanofibers. Taken together, the scaffolds based on controllable aligned electrospun nanofibers show great potential as artificial skin substitutes and may be particularly useful as biomedical patches or grafts to induce wound closure and/or tissue regeneration.

Poster Presentation : **INOR.P-160**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Development of nanodiamonds based multifunctional biosensors

Yoobeen Lee, Jin Seok Lee[*]

Department of Chemistry, Hanyang University, Korea

Nanodiamonds (NDs) have excited a lot of interest in the field of biomedical application as they can be used as spin probes for optical magnetic sensing of cellular and biological environments. Due to their optical and biological properties, NDs are expected to be employed as multitasking markers for the accurate visualization of biophysical parameters such as and magnetic fields and temperature. However, the engineered NDs to intracellular structures of interest within a complicated biological environment remains a challenge. In this research, we investigated each property of the 4 types of nanodiamonds like SEM, PL spectra and then the NDs were transfected into human skin cells (WS1) using silicon nanopillar. For the development of nanodiamonds as multifunctional biosensor, researchers are still engaged in the in-depth study of NDs and their effect on life interfaces.

Poster Presentation : **INOR.P-161**

Inorganic Chemistry

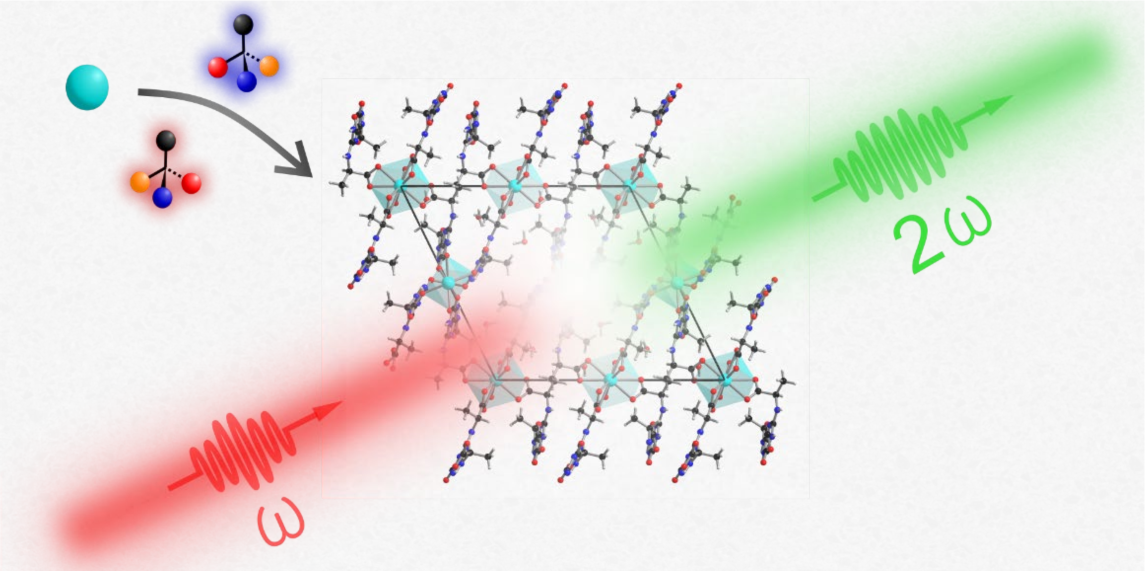
Zoom 3 WED 17:30~18:00

Synthesis, Crystal Structures, and Characterization of Novel Enantiomorphic Lanthanide-based Metal-Organic Frameworks

Yunseung Kuk, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Recently, chiral metal-organic frameworks (CMOFs) have been of great interest because of their intriguing properties such as second-harmonic generation, ferroelectricity, piezoelectricity, pyroelectricity, and chiral properties. However, the preparation of MOFs with non-centrosymmetric (NCS) structures is a highly challenging task because most of solid-state materials with extended frameworks prefer to crystallize in thermodynamically stable centrosymmetric structures. In order to prepare MOFs with macroscopic NCS structures more systematically, novel chiral organic ligands were carefully designed and synthesized. By introducing the chiral linkers, two new lanthanide-based CMOFs have been successfully synthesized through solvothermal reactions. The structures of Ln-MOFs (Ln = La^{3+} and Ce^{3+}) were determined by single crystal X-ray diffraction. The title compounds crystallized in the monoclinic NCS space group, $C2$ attributable to the introduced chiral organic ligands. In this presentation, synthesis, structure determination, and characterizations of the newly synthesized CMOFs are represented.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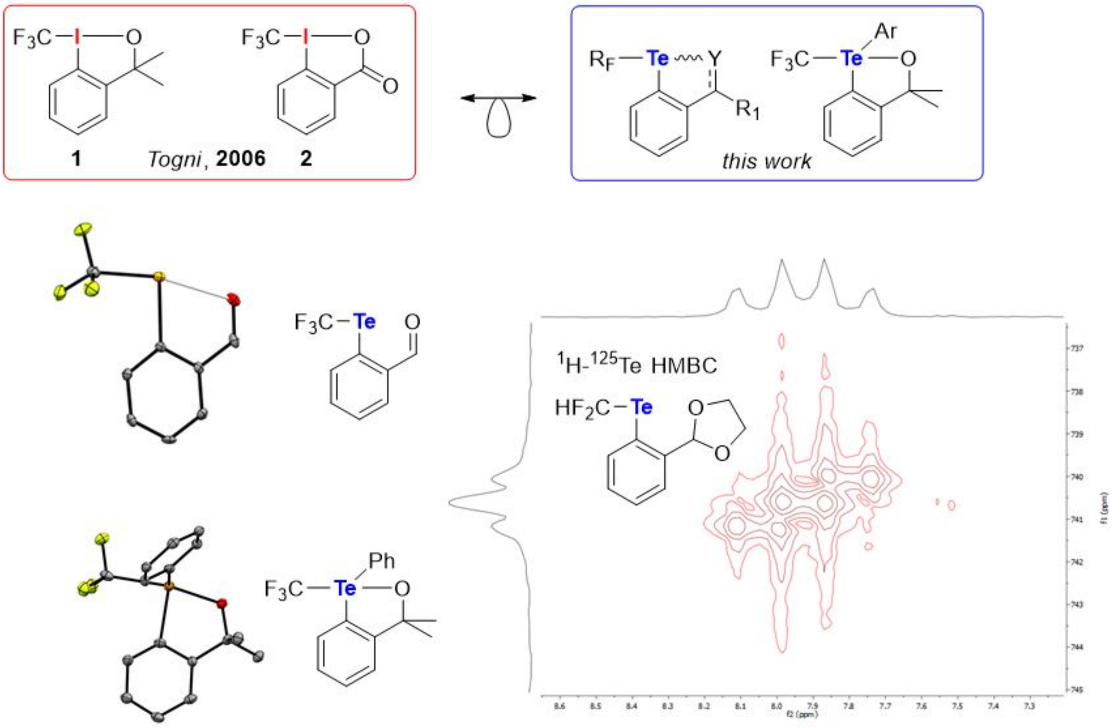
Poster Presentation : **INOR.P-162**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Synthesis and NMR Spectroscopy of Tellurium CF_3 Compounds Isolobal to Iodine(III) Reagents

Ewa Pietrasiak, Antonio Togni[1,*]

Department of Chemistry and Applied Biosciences, ETH Zurich, Poland
[1]*Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland*

Iodine(III) CF3 reagents, commonly referred to as “Togni reagents”, attracted considerable attention not only as efficient electrophilic trifluoromethylating agents but also in the context of structure and bonding in main-group element compounds.1 Herein we present isolobal organotellurium compounds obtained by a formal replacement of the iodine by a tellurium atom. Tellurium(II)2 as well as tellurium(IV)3 derivatives were obtained on gram scale and structurally characterized by multinuclear NMR and single crystal X-ray diffraction. In the case of tellurium(II) compounds, two major synthetic approaches allowing the installation the CF3 (or RF) group on the tellurium atom were developed, by the use of electrophilic CF3I or nucleophilic TMSCF3 (or TMSRF), respectively. Factors determining the 125Te NMR chemical shifts of these compounds were studied by density functional theory (DFT).4 The analysis indicated that the variation in 125Te chemical shifts is mainly due to the magnetic coupling of the tellurium p-character lone pair with antibonding orbitals perpendicular to it upon action of an external magnetic field. Tellurium(IV) compounds were obtained in a three step sequence starting from a thermally induced reaction between an iodine(III) reagent and a ditelluride. The products are bench stable solids, however splitting of the CF3 group to a fluoride and difluorocarbene was observed upon heating in solution. 1. J. Charpentier, N. Früh, A. Togni, Chem. Rev. 2015, 115, 650–682.2. E. Pietrasiak, A. Togni, Organometallics 2017, 36, 3750–3757.3. E. Pietrasiak, A. F. Baxter, B. Jelier, N. Santschi, A. Togni, Helv. Chim. Acta 2019, 102, e1900079.4. A. Togni, C. Coperet, E. Pietrasiak, C. P. Gordon, Phys. Chem. Chem. Phys. 2020, 22, 2319-2326.


F$_3$C–I–O
1
Togni, 2006
2
R$_F$–Te ~ Y
R$_1$
Ar
F$_3$C–Te–O
this work
F$_3$C–Te
O
Ph
F$_3$C–Te–O
^{1}H-^{125}Te HMBC
HF$_2$C–Te
O
O
f2 (ppm)
f1 (ppm)

Poster Presentation : **INOR.P-163**

Inorganic Chemistry

Zoom 3 WED 17:30~18:00

Chemical Patterning in Single Crystals of Metal–Organic Frameworks by Photo-Cycloaddition Reaction in a Single-Crystal-to-Single-Crystal manner

In-Hyeok Park, Eunji Lee[1], Shim Sung Lee[2,*], Jagadese J. Vittal[3,*]

Graduate School of Analytical Science and Technology, Chungnam National University, Korea
[1]*Department of Chemistry, Gangneung-Wonju National University, Korea*
[2]*Department of Chemistry, Gyeongsang National University, Korea*
[3]*Department of Chemistry, National University of Singapore, Singapore*

Metal-organic framework (MOFs) structures are known to exhibit unusual structural flexibility in response to exchange of guest molecules present in the voids. Here we demonstrate that the guest solvent molecules in the voids have a great influence on the outcome of the solid state photochemical reactions in three highly strained Cd(II) MOFs with cds topology [1]. In the railroad track-like [Cd2(bpe)2] chains of the three MOFs, the olefin bond pairs in the bpe (4,4'-bipyridylethylene) ligands undergo photochemical [2+2] cycloaddition reaction under UV light in a single-crystal-to-single-crystal (SCSC) manner. For instance, partial photoreaction in two MOFs with no guest solvent and DMA respectively led to the formation of two photoproducts, ABAB type and AABBAABB type (where A and B are unreacted bpe pairs and cyclobutane rings, respectively). Surprisingly, the MOF with DMF lattice solvent undergoes 100% photoreaction but leading to the photoproduct with broken chains of [Cd2(rctt-tpcb)2] that resembles damaged railroad track. In other words, the strain created by the quantitative formation of cyclobutane rings, is released by breaking one of the rails. More interesting examples are waiting to be explored in the future to underline the role played by the guest solvents on the physical and chemical properties of MOFs.

Poster Presentation : **INOR.P-164**

Inorganic Chemistry

Zoom 3 WED 17:30~18:00

Indol-2-ylidene (IdY): New Generation of N-heterocyclic Carbene – Ambiphilicity, Simple Preparation, Scalability and Tunability

Hyunho Kim, Minseop Kim, Eunsung Lee*

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

Recently, cyclic (alkyl)(amino)carbenes (CAACs) are receiving remarkable attention because of their ambiphilic property. CAACs have high HOMO (higher nucleophilicity, more σ-donating) and low LUMO (higher electrophilicity, more π-accepting) energy level. This small HOMO-LUMO energy gap facilitates the smaller singlet-triplet (S/T) gap. This small S/T gap is a dominant factor for high reactivity of NHCs with inert small molecules such as carbon monoxide. Thanks to this ambiphilicity, CAAC has been applied to diverse fields such as transition metal catalysis and main group chemistry.In the same vein, many kinds of ambiphilic NHCs are developed such as CAAC family, cAArC, cArAmC, and coumaraz-2-on-4-ylidene. However, to the best of knowledge, indole based NHCs were not developed yet. Indole moiety is a promising candidate for ambiphilic NHCs, because indole has cyclic (alkyl)(amino) fragment like CAAC family and also has an aryl group like cAArC and cArAmC. These ambiphilic NHCs exhibited special reactivity such as exchange reactions at main group elements, and [2+1] cycloaddition with dimethyl maleate or fumarate. Furthermore, the synthetic method for the indole moiety is also studied well, because the indole structure is one of the common N-heterocycle found in drug molecules, enzymes, and natural products. It is expected that various indole derived NHCs can be developed through these vast synthetic methods. To explore the ambiphilic potential and synthetic utility of indole derived ambiphilic NHCs, we designed 'Indol-2-ylidene (IdY)'.

Poster Presentation : **INOR.P-165**

Inorganic Chemistry

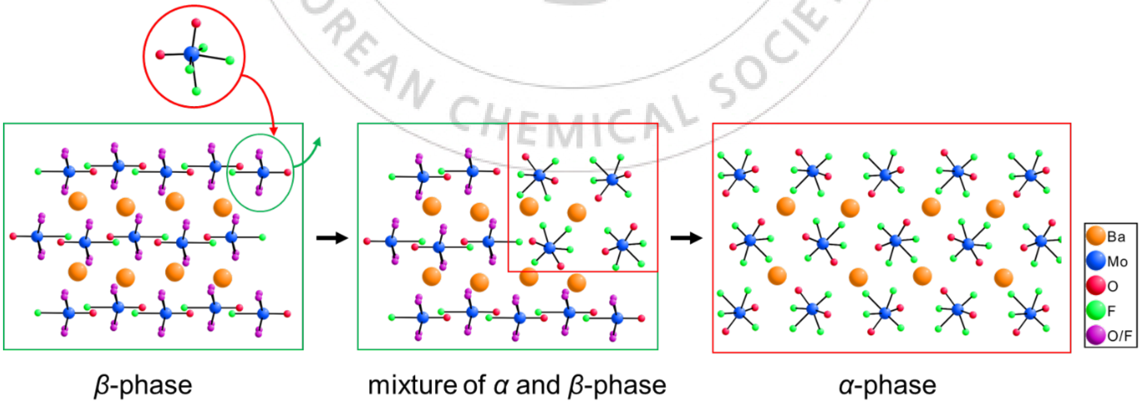
Zoom 3 WED 17:30~18:00

Kinetic study of molybdenum oxyfluorides polymorphs

Hongil Jo, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Two polymorphs of new molybdenum oxyfluorides have been synthesized. A kinetic compound (*β*-phase) is formed first and then a gradual structural change results in a thermodynamically stable compound (*α*-phase). The structures of *α*-phase and *β*-phase were determined by single crystal and powder X-ray diffraction, respectively. The structural analysis indicates that while the *α*-phase and crystallizes in the noncentrosymmetric space group, $Pca2_1$, *β*-phase crystallizes in the centrosymmetric space group, *Cmcm*. The kinetic data are well-fitted with the Avrami equation, which implies that the transformation reaction occurs by an exchange reaction. Other characterizations such as spectroscopic analysis and DFT calculations are also presented.



β-phase mixture of *α* and *β*-phase *α*-phase

Poster Presentation : **INOR.P-166**

Inorganic Chemistry

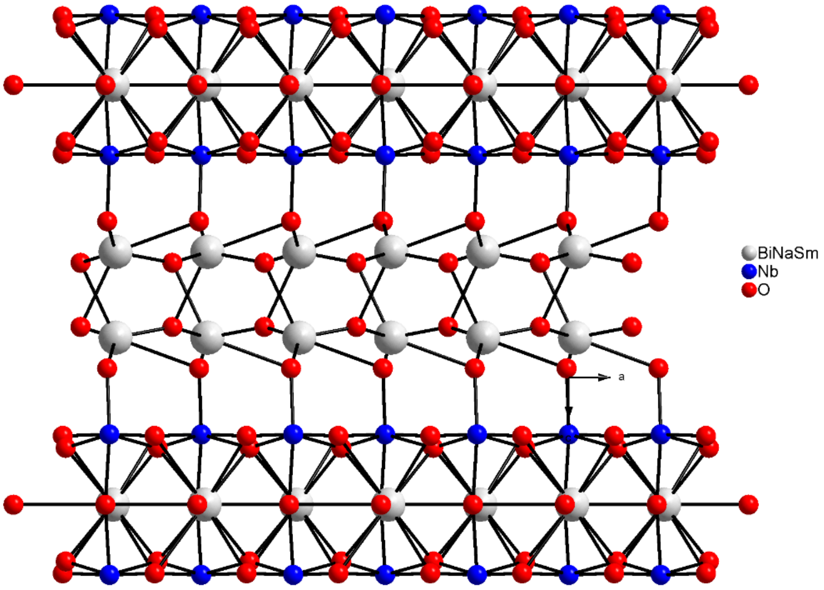
Zoom 3 WED 17:30~18:00

Synthesis, Crystal Structures, and Characterization of a Series of Aurivillius-type Perovskites

Kisung Kim, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Perovskite, an attractive subject in many research areas, has been well-known for its multifunctionality. Especially, perovskites with noncentrosymmetric (NCS) structure are of great interest for the unique characteristics such as ferroelectricity, piezoelectricity, and nonlinear optical (NLO) properties. One of the NCS perovskites, $Na_{0.5}Bi_{2.5}Nb_2O_9$ with a polar structure is expected to have interesting NLO properties. Since it has been studied only on phase transition and other electrical properties, we have investigated a more detailed NLO property changes by substituting lone pair cations with lanthanide elements. The doped compounds have been successfully synthesized by solid state reactions. The crystal structures were determined by the Rietveld refinement. Crystal structures and characterizations of the reported compounds are presented.


BiNaSm
Nb
O
a

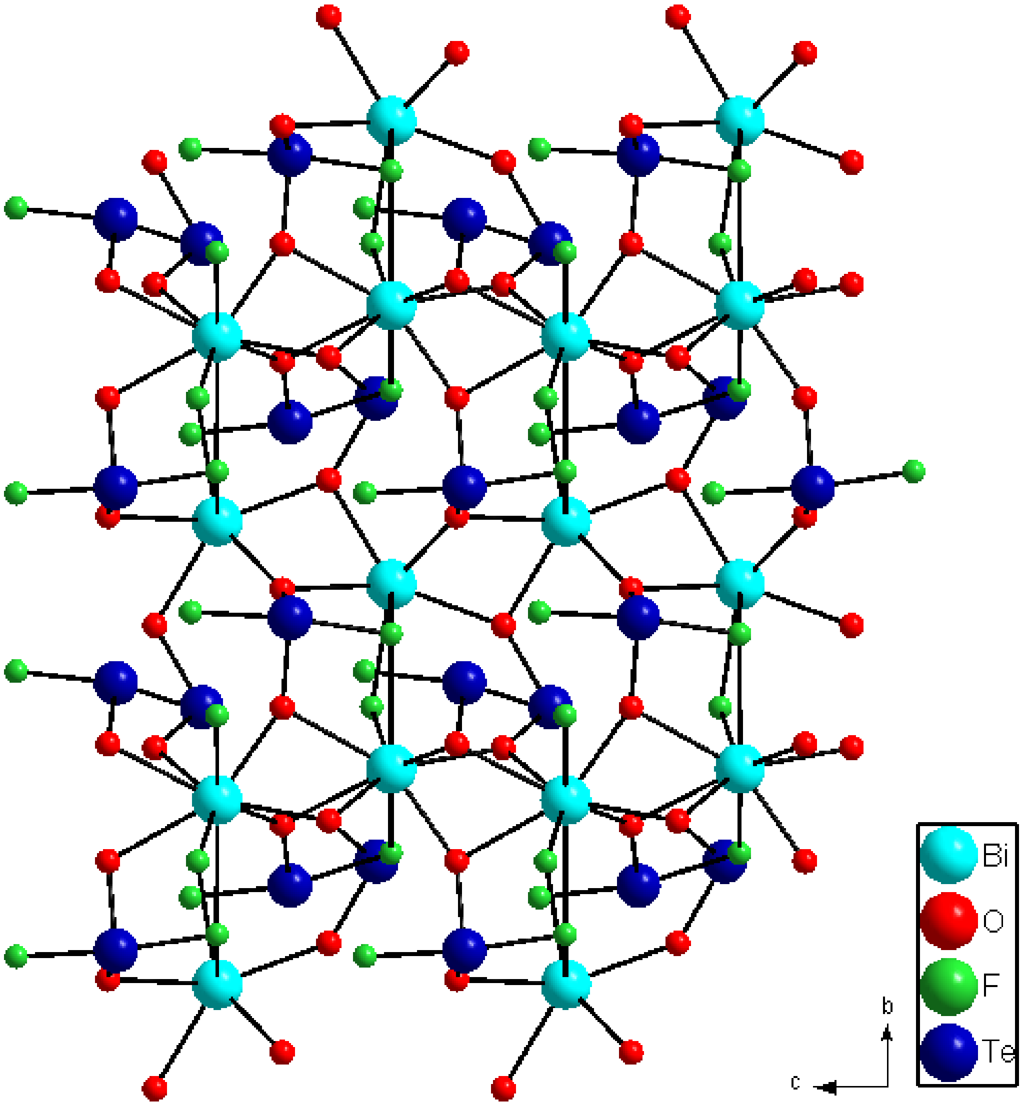
Poster Presentation : **INOR.P-167**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Synthesis and Characterization of a New Bismuth Tellurite

Jee Yoon Chung, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

We have synthesized a new bismuth tellurite through a hydrothermal reaction. Single crystal X-ray diffraction indicates that the novel bismuth tellurite crystallizes in the polar hexagonal space group, $P6_3mc$. The compound reveals a three-dimensional structure consisting of BiO_6F_3, TeO_3, and TeO_2F_2 groups. Energy dispersive X-ray spectroscopy demonstrates that the title compound is composed of Bi, Te, O, and F, and the composition is consistent with the crystallographic result. Bond valence sum data of the reported compound match well with the expected charge of each element. The result of local dipole moment calculations is also presented.


Bi
O
F
Te
b
c

Poster Presentation : **INOR.P-168**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Metal-based complexes for multidrug-resistant pathogens: Synthesis, characterization and biological applications

Getinet Tamiru[*], **Atakilt Abebe**[1], **Moges Abebe**[1], **Misganaw Liyew**[1]

Chemistry Department, Science College, Bahir Dar University, Ethiopia
[1]*Bioinorganic Chemistry, Science College, Bahir Dar University, Ethiopia*

Background: The intensive use of antibiotics has led to an increase in drug-resistant bacteria against known antibiotics. To overcome the alarming problem of microbial resistance to antibiotics, the discovery of novel active compounds against new targets is a matter of urgency. Based on this, we report, three new mixed ligand complexes of cobalt(II) viz. mononuclear ([Co(phen)2(Act)(H2O)]Cl2.H2O and [Co(phen)2(Act)(en)]Cl2), and binuclear [Co2(phen)4(Act)2(en)]Cl4 which were synthesized from CoCl2.6H2O, 1,10-phenanthroline monohydrate, acetamide, and ethylenediamine.

Method: In the first step, the precursor complex was synthesized from cobalt chloride salt and 1,10-phenanthroline, then the precursor complex was treated with acetamide to give the [Co(phen)2(Act)(H2O)]Cl2.H2O complex. Finally, the ([Co(phen)2(Act)(H2O)]Cl2.H2O complex was treated in different stoichiometry separately with one and two moles of ethylenediamine resulting the corresponding mononuclear and binuclear Co(II) complexes, respectively. All the complexes were synthesized in methanol media, through refluxing under controlled reaction conditions. The synthesized complexes were characterized using spectroscopic (ESI-MS, ICP-OES, FT-IR, and UV-Vis), chloride determination as well as melting point and conductance measurement. In vitro antibacterial activity was also tested on two Gram-positive (Staphylococcus aureus, Streptococcus pyogenes) and two Gram-negative (Escherichia coli and Klebsiella pneumoniae) bacteria using the disc diffusion method and compared with the standard commercially available drug, Gentamicin.

Results: All the synthesized Co(II) complexes were proposed octahedral geometry and showed moderate to high antibacterial activity. The complexes demonstrated appreciable activity even against the Gram-negative bacteria. The antibacterial result was found comparable with the commercial drug Gentamicin even at a lower concentration of complexes.

Conclusion: The results indicated that the synthesized complexes may be considered as potential antibacterial agents after passing cytotoxicity testing.

Poster Presentation : **INOR.P-169**

Inorganic Chemistry

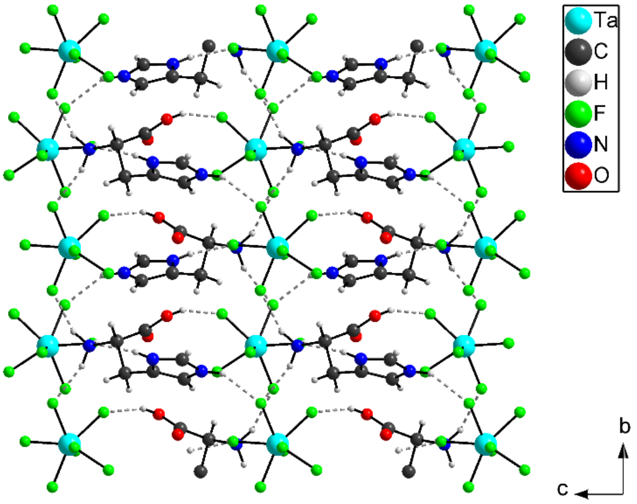
Zoom 3 WED 17:30~18:00

Synthesis, crystal structures, and characterization of the new noncentrosymmetric histidinium tantalumfluoride

Heejung Choi, **Kang Min Ok**[*]

Department of Chemistry, Sogang University, Korea

Since most of the solid-state materials preferred centrosymmetric (CS) structures thermodynamically, introducing chiral molecule on inorganic units is an effective pathway to discover new macroscopic non-centrosymmetric (NCS) structures systematically. New enantiomorphic histidinium tantalum fluoride compounds have been successfully synthesized through slow evaporation method and their structures were determined by single crystal X-ray diffraction (SC-XRD). The structures of the title compounds are composed of L- or D-histidinium cations and distorted monocapped trigonal prismatic tantalum fluoride polyhedra. SC-XRD reveals that the materials crystallized in the polar space group, $P2_1$ attributed to the introduced amino acid, histidine. Other characterizations such as spectroscopic, thermal, and elemental analyses will be also provided.


Ta
C
H
F
N
O
b
c

Poster Presentation : **INOR.P-170**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

First-row early transition metal complexes with a highly sterically demanding triisopropylphenyl amino triphenolate ligand: synthesis and applications

Dae Young Bae, Kyung-sun Son[1,*], Eunsung Lee[*]

Department of Chemistry, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Chungnam National University, Korea*

Amino triphenolate ligands have been widely used for the synthesis of various transition metal complexes aiming at various applications such as ring-opening polymerization, olefin polymerization, and sulfoxidation. However, the introduction of highly sterically demanding aromatic substituents, such as triisopropylphenyl (TRIP), to the amino triphenolate ligand has not been previously reported probably due to the synthetic difficulty. In six-step reactions using commercial materials, a highly sterically demanding amino triphenolate ligand was successfully synthesized without column chromatography for purification in each step, and early transition metal complexes (Ti, V, Cr, Mn) supported by the ligand were also obtained and fully characterized. In addition, the titanium complex was further used for catalytic sulfoxidation and formation of a metal hydride complex, and the chromium complex was used for polymerization of ethylene and nitric oxide fixation.D. Y. Bae, G. S. Park, N. Ko, K. Son, E. Lee, Dalton Trans. 2019, 48, 9617. -Reproduced by permission of The Royal Society of Chemistry

Poster Presentation : **INOR.P-171**

Inorganic Chemistry

Zoom 3 WED 17:30~18:00

The control of hydrophobicity upon the uptake of the surfactant into the supramolecular inner cavity

Haeri Lee[*], **Ok-Sang Jung**[1]

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

The purpose of the construction of a flexible supramolecular frame is for the use of their inner cavity as a selective molecular recognition for molecular storage and a delivery system. The skeletal structures of supramolecular coordination compounds constructed via metal-mediated self-assembly can interact with guest molecules by weak interactions such as electrostatic attractions, van der Waal interactions, and hydrogen bonds. The main driving force for the formation of host-guest complexed bound between charged hosts and charged guests is electrostatic attractions. Herein, we present an unprecedented novel approach to the control of the uptake of alkyl sulfate surfactants based on flexible host–guest interaction between alkyl sulfates and large coordination cages. For the aggregates encapsulated via hydrogen bonds between sulfate groups and cage skeletons, the contact angles were measured according to the length of the alkyl sulfates. Electrostatic interaction between $Pd^{2+}\cdots{}^{-}OSO_3R$ (R=ethyl, octyl, decyl, dodecyl, tetradecyl) (3.92(1)–4.23(2) Å) forced to face each other inside cage.

Poster Presentation : **INOR.P-172**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

Understanding the adsorption mechanism of methyl iodide on functionalized Ag nanoparticle-embedded and Ag^+ ion coated silica gels

Jeong Woo Hong, Hee-Jung Im*

Department of Chemistry, Jeju National University, Korea

To detect iodine in the air, silica gels functionalized by ethylenediamine and mercapto were prepared. Each of these functionalized silica gels was put in isopropanol solution in which $AgNO_3$ was dissolved. After then, the solutions containing silica gels were irradiated with an electron beam or left unattended to produce Ag nanoparticle-embedded functionalized silica gels (Ag NP) and Ag^+ ion-coated functionalized silica gels (Ag^+). All prepared silica gels were exposed to methyl iodide gas (; mixed with high purity air) to investigate the mechanism how methyl iodide interact to the prepared silica gels and the tendency of methyl iodide to be adsorbed. Diverse spectroscopic analyses were applied to distinguish and explain the differences according to the silvers (Ag NP, Ag^+) and groups (ethylenediamine, mercapto).

Poster Presentation : **INOR.P-173**
Inorganic Chemistry
Zoom 3 WED 17:30~18:00

SuFEx-based Post-synthetic Modification of Metal-organic Frameworks

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. Among various methods, post-synthetic modification (PSM) strategies have been mainly utilized to introduce novel properties in the MOFs.[1] The first option to introduce the property is to modify the organic linkers. Recently, a new type of PSM strategy utilizing sulfur(VI) fluoride exchange (SuFEx),[2] was reported.[3] With this method, several functional groups were successfully substituted with high yields. Here we report two new MOFs with sulfonyl fluoride that is possible for PSM via SuFEx. They are successfully characterized by SXRD, PXRD, and gas sorption. Currently, the applications using these materials are in development. In addition, SuFEx with several catalysts for PSM is investigated.Reference[1] Cohen, S. M., *J. Am. Chem. Soc.*, **2017**, 139, 2855.[2] Dong, J.; Krasnova, L.; Finn, M. G.; Sharpless, K. B. *Angew. Chem. Int. Ed.*, **2014**, 53, 9430.[3] Park, S.; Song, H; Lee, E. *et al ACS Appl. Mater. Interaces*, **2018**, 10, 33785.

Poster Presentation : **INOR.P-174**

Inorganic Chemistry

Zoom 3 WED 17:30~18:00

Symmetry-guided evolution of *de novo* metallo-β-lactamases

Jaeseung Yu, **Woon Ju Song**[1,*]

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

Directed evolution has yielded numerous novel bio-catalysts by mimicking natural evolution process in the laboratory. However, the adequate selection of evolution targets and the effective construction and screening of the mutant libraries still remain elusive. We herein suggested that protein symmetry can serve as a novel criterion to seek promising hotspots for protein evolution. We carried out iterative saturation mutagenesis of four symmetry-related residues located at rotation axes of *de novo* metallo-β-lactamase. The optimization of symmetry-related residues provided a significant effect in catalytic activities, while those of proximal residues exhibited trivial alterations. The identification and *in vitro* characterization of positive hits suggested that symmetry-guided evolution can yield considerable alterations in overall structures, metal-coordination geometry, and chemical environments of the active sites. Iterative evolution during four rounds produced high catalytic enhancement from the parent protein.

Poster Presentation : **PHYS.P-175**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Behaviors of halloysite nanotubes in polymer electrolytes: poly(styrene sulfonate) and poly(allylamine)

Jungju Ryu, **Daewon Sohn**[1,*]

Department of Chemistry and Research Institute for Convergence of Basic Sciences, Hanyang University, Korea

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

Halloysite clay nanotubes have great attention due to the promising applications such as drug delivery, chemical carriers, and biomaterials. These tubular particles have various spaces that can allow to load substances with sizes from atomic to molecular levels. Even though they have a lot of benefits, their surface charges close to neutral states generate aggregation that limits further improvement for the applications. Therefore, there have been many efforts to improve their dispersity by controls of solvent quality and by addition of surfactants. However, it has been still veiled about solution characteristics that address how to diffuse and interact. In this study, we investigated halloysite solutions upon pH, salt, and polyelectrolyte, in order to know in-situ behaviors of the particles. Polarized/depolarized light scattering revealed diffusion of a single nanotube in high pH condition, and also these nanotubes were probed in solutions with two different polyelectrolytes, anionic and cationic polymers (poly(styrene sulfonate) and poly(allylamine)) by using small angle X-ray scattering. We observed chain conformational characteristics upon concentrations of polyelectrolytes and discussed depletion stabilization and depletion flocculation that support the particle stability. This study improves the knowledge about halloysite behavior and provides the insights to develop novel materials using halloysite tubes.

Poster Presentation : **PHYS.P-176**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Simulation of the Magnetic Weight Increase by Agglomeration Dynamics of Magnetic Nanoparticles under Magnetic Field using Boltzmann Distribution Function

Hackjin Kim

Department of Chemistry, Chungnam National University, Korea

Agglomeration of the magnetic nanoparticles under the magnetic field has been studied by monitoring the magnetic weight of the sample. The magnetic weight measured with the electronic balance is the magnetic force that the magnetic sample experiences under the magnetic field. The magnetic weight of the superparamagnetic magnetite nanoparticles in aqueous solution increases slowly. The overall increase of the magnetic weight follows the stretched exponential function, which results from the distribution of the energy barrier of the dynamics. The inhomogeneity of the nanoparticles of the sample makes the distribution of the energy barrier involved in the dynamics. The time dependence of the dynamics is given by the Laplace transform of the distribution of the rate constant, which results from the distribution of the energy barrier. The Boltzmann distribution is employed for the simulation of as the first trial, which is the simple but the physically reasonable distribution function. The simulation results fit well with the stretched exponential function in the early stage of the dynamics. With the increase of the simulation time, the fitting becomes poor but not so bad. The exponent of the stretched exponential function becomes smaller with the increase of the simulation time, which is physically correct. As the dynamics spans longer time, new channels with different energy barriers contribute to the dynamics, therefore, the exponent becomes smaller.

Poster Presentation : **PHYS.P-177**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Effects of alkali ion-doping on diffusion mechanisms and thermal stabilities of imidazolium-based organic ionic plastic crystal

Chung Bin Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

There have been efforts to replace lithium ion batteries to sodium ion batteries due to lithium dendrite problem at the electrode and unstable solid electrolyte interface (SEI) problem. In case of organic ionic plastic crystal (OIPC), which is the new class of solid electrolyte, the alkali doping also matters for two reasons. One is thermal stability and the other one is higher ionic conductivity. In this work, we perform molecular dynamics simulations to investigate effects of alkali ion doping on rotational and translational diffusion of ions and melting temperatures of OIPC. In our simulations, we employ lithium ion (Li^+), sodium ion (Na^+), and potassium ion (K^+) as doping agents on 1- methyl-3-methylimidazolium hexafluorophosphate ($[MMIM][PF_6]$). From our results, the smaller size of alkali ion is doped, the more lattice structure gets distorted. As larger distortion disable the crystal to maintain its lattice structure, Li^+ doped crystal shows lowest melting temperature. The size of alkali ion also affects rotational diffusion of $[MMIM]^+$ (or PF_6^-). $[MMIM]^+$ (or PF_6^-) shows highest rotational disorder when Li^+ is doped. Not only the rotational diffusion, but also translational diffusion mechanism of alkali ions are different depending on the kind of doped alkali ion. Li^+ shows continuous diffusion through amorphous regimes, whereas K^+ shows the hopping diffusion. Na^+ shows intermediate feature of diffusions between Li^+ and K^+.

Poster Presentation : **PHYS.P-178**

Physical Chemistry

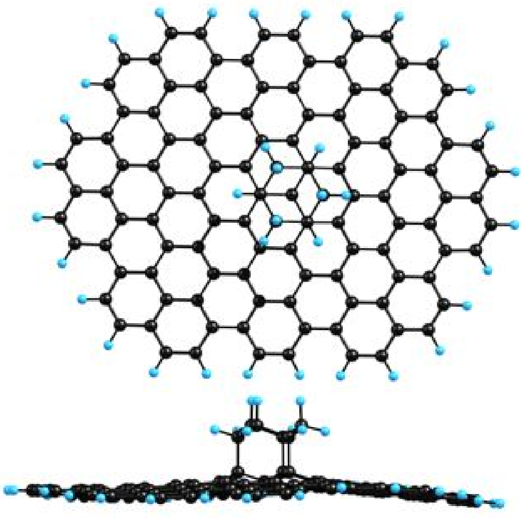
Zoom 4 WED 16:30~17:00

Formation of Quantum Antidot Superlattices

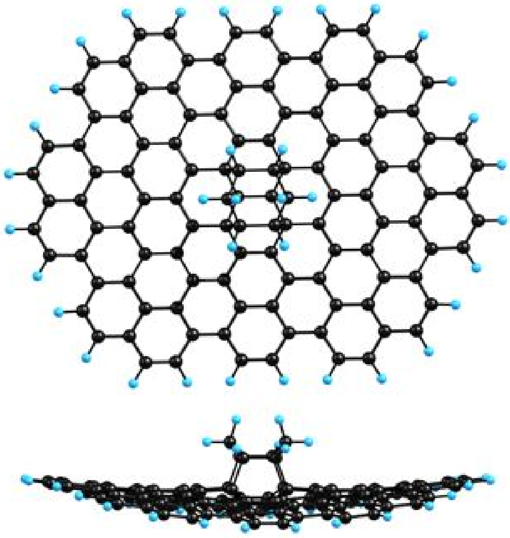
Gbenga Oyeniyi

chemistry, kyungpook national university, Nigeria

We report results of first principle density functional theory calculations, which introduces a new possibility of carbon nanostructures that can be formed due to the adsorption of benzene (aromatic) on the external surface of a single layer of a graphene sheet. This forms an ultrathin diamond film on the surface due to the creation C-C covalent bond. This ultrathin diamond film can be formed by chemical functionalization on the surface of the single-layer graphene sheet supported by a substrate (e.g. SiC). The two different possible conformations of these two ultrathin diamond films can be a cubic diamond film (111) or a hexagonal diamond film (1010). We find that this unique nanostructure has fascinating electronic properties with bandgap which can cane used as an antidote material. We performed the geometry optimization on armchair-edged bilayer superlattices graphene nanosheet within 2.2nm with different sides. Both nanostructure conformations were optimized at PBE0/6-31G*, as implemented in GAMESS. We assumed that this nanomaterial could be formed by employing the Plasma Enhanced Chemical Vapour Deposition and Spark Plasma Sintering (SPS).



Cubic diamond film (111)



Hexagonal diamond film (1010)

Poster Presentation : **PHYS.P-179**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Development of a new approach for ultralow-laser-power STORM imaging

Jin Kyoung Chung, Doory Kim*

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 fluorophores. In principle, the super-resolution of STORM can be obtained by high-accuracy localization of photo-switchable fluorophores, which requires fast photo-switching and bright fluorescence intensity from a single emitter. It is known that the switching rate of photo-switchable fluorophores shows laser power dependency and the high laser power is required for the enhancement of imaging resolution. However, high laser power required is usually harmful to live biological specimens due to its photo-bleaching effects and high photo-toxicity. Here, we attempted to overcome this issue by improving the STORM resolution at a lower laser power. Through the quantitative analysis of photo-switching behavior of single fluorophores under different laser power conditions, we develop a new approach to achieve super-resolution fluorescence images even with much lower power than before. This approach is expected to play an increasingly significant role in super-resolution live-cell imaging using STORM.

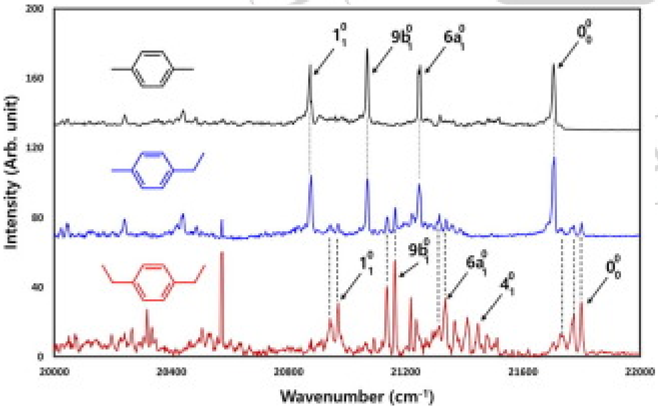
Poster Presentation : **PHYS.P-180**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Spectroscopic identification of the p-ethylbenzyl radical in a corona-excited supersonic expansion

Changsoon Huh[*], Yu Jin Song

Department of Applied Chemistry, Dong-Eui University, Korea

The excitation spectrum of the jet-cooled p-ethylbenzyl radical was generated from the precursor 1,4-diethylbenzene in a corona-excited supersonic expansion (CESE). Assignment of the p-ethylbenzyl radical was confirmed by comparing the spectra from p-xylene and p-ethyltoluene. The geometry optimization and vibrational frequencies of the p-ethylbenzyl radical were computed with density functional calculation. Conclusive vibronic band assignment was analyzed with a Franck-Condon simulation in the D0 − D1 transition.



Poster Presentation : **PHYS.P-181**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Evolutionary Conservation of Amino Acids Contributing to the Dynamic Cooperativity in Protein Folding

Song-Ho Chong, Sihyun Ham*

Department of Chemistry, Sookmyung Women's University, Korea

Evolutionary conservation of amino acids critical to protein folding, typically judged by the Phi-values, has been investigated intensively in the past. However, no consensus has yet been reached. Here, we investigate this issue in terms of the dynamic cooperativity. We find a strong indication of a new kind of relationship – necessary but not sufficient causality – between the evolutionary conservation and the dynamic cooperativity: Larger contributions to the dynamic cooperativity arise from more conserved residues, but not vice versa. To the best of our knowledge, this is the first demonstration of any kind of evolutionary conservation of amino acids relevant to folding kinetics.

Poster Presentation : **PHYS.P-182**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Structural and thermodynamic factors responsible for early inherent aggregation tendency of monomeric Tau43

Prathit Chatterjee, Sihyun Ham[*]

Department of Chemistry, Sookmyung Women's University, Korea

Recent studies in the field of Alzheimer's disease (AD) investigated the precise mechanisms leading to the formation of neurofibrillary tangles (NFT) and senile plaques. NFTs, the aggregated Tau protein isoforms, are one of the primary factors behind AD. The minimal sequence of human Tau protein variant Tau43 or PHF43 (a 43-residue Tau fragment), as paired helical filaments (PHFs), has been found to self-assemble into pathological diseased aggregates. However, the molecular details in rationalizing the aggregation propensity of Tau43 remain elusive. Herein, using atomistic, explicit water molecular dynamics simulations and subsequently solvation thermodynamic analyses on aqueous Tau43, we identify the molecular factors responsible for the critical behavior of PHF6 (VQIVYK) fragment in facilitating Tau43 aggregation in water. The segment, although showing no specific secondary structural affinity within the simulated timescales, exhibit more thermodynamic instability factors, relative to other domains. The corresponding potential aggregation propensity is therefore inherently seeded in it. Further, the transient hydrogen bonds formed involving the positive residues of N-terminal and C-terminal E43, are relatively shielding this segment, from being totally exposed to water, thereby potentially responsible for corresponding positive solvation thermodynamic contribution. These findings will lead to consecutive investigations for a detailed understanding of the AD pathway, eventually guiding in corresponding drug designing avenues for the prevention of AD progression.

Poster Presentation : **PHYS.P-183**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Orbital asymmetry in dissociative electron attachment to several trihalobenzenes using effective core potential

Jangho Park, Namdoo Kim[*]

Chemistry, Kongju National University, Korea

“Orbital asymmetry” in atomic selectivity is originated from asymmetric participation of molecular orbitals in a reactive collision. Previously, we investigated dissociative electron attachment to dihalobanzenes. We now expand our territory to benzene molecules with three halogen atoms. Trihalobenzenes like 1,3-dichloro-2-bromobenzene (DCBB), 1,3-dibromo-2-iodobenzene (DBIB), 1,3-dichloro-2-iodobenzene (DCIB) were studied theoretically using DFT calculation. For iodine containing molecules, DBIB and DCIB, efficient core potential (ECP) was considered for iodine. In conclusion, structure and energy are almost the same for both cases, ECP-considered and non-considered. Iodine is dissociated from DCIB, DBIB while bromine is dissociated from DCBB upon electron attachment. We figured out that an approaching electron is mostly localized to the less electronegative halogen atom from Mülliken charge analysis. In addition, anti-bonding orbital between halogen and carbon atom has atomic character of less electronegative halogen atom leading to increase of the bond length.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

Zoom 4 WED 16:30~17:00

The effect of surface roughness and heating treatment on sputtering yield

Tae Hyun Kwon, Sangjune Park, Young-Sang Youn[*]

Department of Chemistry, Yeungnam University, Korea

Fusion power has been attracting an attention because it could be possible to use the source of alternative energies for fossil fuels. One of the main issues for nuclear fusion is how to preserve the high temperature plasma for nuclear fusion reaction. Tungsten is one of the candidates for use as a plasma facing materials in the diverter of a nuclear fusion reactor because of its low hydrogen retention and high melting temperature compared to the others.Previous research reported that the sputtering yield for tungsten is influenced by its surface roughness [1]. If the impurities generated by sputtering phenomenon on tungsten surface are injected into the plasma, the temperature of the plasma will decrease by them, leading to the decrease in the performance of the nuclear fusion reactor. Therefore, the sputtering yield for tungsten must be reduced to prevent the degradation for its performance.In this study, we investigated the effect of surface roughness and heating treatment on sputtering yield of tungsten. On the basis of the experimental data, we confirmed that the sputtering yield for a tungsten pellet consisting of large powder size is lower than that composed of small powder size, resulting from that the increase in tungsten powder size gives rise to the increase in surface roughness of the tungsten pellet. In addition, we found that the sputtering yield of the tungsten pellet treated the heating up to 500 °C gradually decreases, which could be due to the increase in its crystallite size.[1] D. Nishijima et al., J. Nucl. Mater. S96-S99 (2011) 415

Poster Presentation : **PHYS.P-185**

Physical Chemistry

Zoom 4 WED 16:30~17:00

The effect of chemical reagent on photo-switching property of fluorescent organic dyes for super-resolution imaging

Seokran Go, Hyunbum Park, Doory Kim*

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Recent years have witnessed the rise of super-resolution fluorescence microscopy as a key tool to study biological ultrastructures. In particular, STORM relies on the localization of single fluorescent molecules by using photo-switching of individual molecules within the diffraction-limited region at different times. It has been reported that the reactivity of the thiol in imaging buffer plays a key role in the photo-switching process. Based on this hypothesis, here, we tested various chemical reagents for a dye reaction by quantifying their photo-switching properties. Through this test, we demonstrate that various chemical reagents which form a covalent adduct with fluorescent organic dye can be used for super-resolution imaging.

Poster Presentation : **PHYS.P-186**

Physical Chemistry

Zoom 4 WED 16:30~17:00

D-glucuronic acid-coated mixed Zn(II)/Gd(III) oxide nanoparticles for T_1 MRI Contrasting Agent

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Department of Chemistry, Kyungpook National University, Korea

In this study, we synthesized D-glucuronic acid-coated mixed Zn(II)/Gd(III) oxide nanoparticles (Zn:Gd = ~ 8: ~ 92 in mole percent) were synthesized with d_{avg} of 2.1 nm. We attribute this to reduce the magnetization of the mixed nanoparticles owing to non-magnetic Zn in the nanoparticles. The nanoparticles showed a longitudinal water proton relaxivity (r_1) of 12.3 $s^{-1}mM^{-1}$ with $r_2/r_1 = 1.1$. We characterized particle diameter, hydrodynamic diameter, surface coating, magnetic properties, cellular cytotoxicity, water proton relaxivities, and in vivo T_1 MR Images. Highly positive contrast enhancements were observed in T_1 MR Images of a mouse.

Poster Presentation : **PHYS.P-187**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Unveiling Interfacial Charge Recombination Dynamics in Colloidal Quantum Dot Photovoltaics with Polymeric Hole Transport Layers

Jonghee Yang, Whikun Yi*

Department of Chemistry, Hanyang University, Korea

The state-of-the art PbS colloidal quantum dot photovoltaics (CQDPVs) now exhibit promising performances toward next-generation solar cell, recording the highest power conversion efficiency (PCE) nearly 14%. Since the charge, particularly hole, collection in these photovoltaics is a key issue toward their high performance, various attempts have been demonstrated to address the issue. Among them, use of polymeric hole transporting layers (HTLs) is regarded as an effective method, since they provide efficient charge transport properties as well as good stability. Recently, we found that the fabrication environment is a key factor determining the performance of CQDPVs: Oxidation of the uppermost CQD surface by ambient oxygen result in an inappropriate chemical and energetic structures for charge transport. Herein, we demonstrate that the oxidation of CQD significantly promotes interfacial charge recombination between the CQD and polymeric HTL by using photoinduced charge extraction by linearly increasing voltage (photo-CELIV) technique. By using the dynamic approach, we observed that both suppression of charge mobility and significant bimolecular recombination occur in the CQDPVs fabricated in air compared with those values obtained from the CQDPVs made in inert atmosphere. In order to solve this, we suggest a novel method to reconstruct the oxidized CQD surface via a chemical post-treatment. This approach not only recovers the oxidized CQD but also effectively passivates the CQD surface, providing a novel and effective platform toward high performance CQDPV as well as the ease of fabrication process.

Poster Presentation : **PHYS.P-188**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Single-molecule spectroscopic study of solvatochromic molecules using spectral STORM

Hyunbum Park, Geun-ho Kim, Doory Kim*

Department of Chemistry, Hanyang University, Korea

The recent development of super-resolution fluorescence microscopy (SRM) allows the location of molecules to be determined with nanometer-scale spatial resolution. The SRM has been recently extended to also capture spectral information of single-molecule with high spatial and spectral resolution. In particular, we have recently developed spectral STORM, which allows us to record the fluorescence emission spectra and positions of ~10^6 single molecules with excellent spectral separation and spatial resolution. By taking advantage of the capability of spectral STORM to resolve in situ the fluorescence emission spectra of single molecules, here we examined the single-molecule fluorescence spectrum changes of various solvatochromic molecules in different environments. Also, we studied the solvent-induced structural modifications of solvatochromic molecules by exploiting a time-dependent density functional theory (TD-DFT) approach coupled with complementary solvation approaches. Such integration has allowed us to achieve a nanoscopic understanding of the solvation effects which govern the absorption and fluorescence properties of solvated molecules, which has not been achieved by conventional spectroscopic methods. Our approach will open the door to the simultaneous nanoscale structural imaging and local sensing of surface and soft-matter systems inaccessible to current methods.

Poster Presentation : **PHYS.P-189**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Construction of 1D TiO_2 nanotube on ultrathin 2D $ZnIn_2S_4$ nanosheets Heterostructure for Photocatalytic CO_2 Reduction

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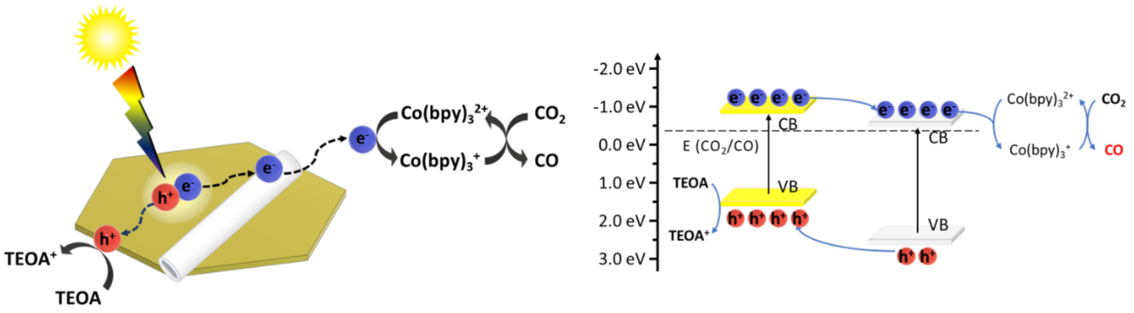
For the past few years, TiO_2 and $ZnIn_2S_4$ have been studied for conversion of CO_2 to generate environmentally friendly chemical energy under solar light. However, there was a restraint because of its poor CO_2 adsorption and charge carrying ability. In this study, TiO_2 nanotube (TNT) is fabricated as TiO_2 nanotube has higher electron mobility and specific surface area. Moreover, it has a wider bandgap around 3.5 eV that reduces recombination of electron-hole pair. To make a further improvement of electron delivery, $Co(bpy)_3^{2+}$ cocatalyst is introduced as it can capture electrons from ZIS conduction band to reduce CO)$_2$. ZIS@TNT composite heterostructure is proved by Mott Schottky measurement and Diffuse reflectance spectroscopy. In this mechanism, photogenerated electrons in the ZIS conduction band are moving to the TNT conduction band, transferred to $Co(bpy)_3^{2+}$. This is reduced to $Co(bpy)_3^{+}$ in turn, which can reduce CO_2 to CO by being oxidized to the original state simultaneously. The optimized ratio of ZIS@TNT (10 wt%) has radically higher CO production than TNT and ZIS themselves. It produces CO with the rate of 4.37 mmol/(g·h), which is 2.6 times faster than that of ZIS. The stability of this material is proved by the long-time photocatalytic reaction. CO production and H_2 production were still continued for 70 hours and more, indicating that ZIS@TNT heterostructure has fine duration under solar light irradiation. This was also shown by 4 times of recycling test, showing almost same activity and selectivity during this experiment.


TEOA⁺
TEOA
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Co(bpy)₃²⁺
Co(bpy)₃⁺
CO₂
CO
-2.0 eV
-1.0 eV
0.0 eV
1.0 eV
2.0 eV
3.0 eV
CB
VB
E (CO₂/CO)
TEOA
TEOA⁺
Co(bpy)₃²⁺
Co(bpy)₃⁺
CO₂
CO

Poster Presentation : **PHYS.P-190**

Physical Chemistry

Zoom 4 WED 16:30~17:00

A comparative study of various spectral STORM spectroscopy techniques

Geun-ho Kim, Hyunbum Park, Doory Kim*

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Recently, single-molecule spectroscopy has become an attractive topic for researchers in various fields. In particular, recently developed spectrally resolved STORM (SR-STORM) allows us to assemble spectral information, together with the super localized positions of the same molecules. To disperse emitted fluorescence of a single fluorescent molecule into a spectrum, various spectroscopic methods can be applied. In this study, we compare the various single-molecule spectroscopy methods by systematically quantifying their spectral, spatial, and time resolution. For this comparative study, the different spectroscopic setups were built on a same microscope as modules, and the measurement of the single-molecule fluorescence spectra obtained from each setup was systematically compared. We anticipate that our study will provide a guideline to apply various single-molecule spectroscopy tools to the study of chemical reactions at the single-molecule level.

Poster Presentation : **PHYS.P-191**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Fe_3O_4@TiO_2-Au Heterostructure as a SERS-active Reusable Photocatalyst

<u>Sila Jin</u>, Lei Chen[1], Young Mee Jung[*]

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Au nanoparticles (Au NPs) are an excellent photocatalyst and surface-enhanced Raman scattering (SERS) active materials. However, Au NPs are easy to aggregate, which easily reduce the photocatalyst and SERS efficiency.In this study, Fe3O4@TiO2 NPs were used as a support material for Au NPs to prevent their aggregation. Proposed Fe_3O_4@TiO_2-Au heterostructure can be reused many times.The fabricated Fe_3O_4@TiO_2-Au heterostructure was characterized by TEM, XRD and XPS. The photocatalytic efficiency was also confirmed by UV-Vis absorption spectrum of methyl orange (MO). In addition, SERS activity and photocatalytic ability at the visible region were examined. Details on its characterization and analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-192**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Local Environment Effects on Enhanced Solubility of Single-Domain Antibodies with Charged Mutations

Jihyeon Lee, Song-Ho Chong[1], Sihyun Ham[1,*]

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Aggregation of antibodies poses severe risks such as poor reproducibility and unwanted immunogenicity in their therapeutic applications. Inserting charged mutations to variable domains is being recognized to be a promising strategy to improve aggregation resistance. However, it remains incompletely understood where (inserting locations) and what type (positive or negative) of mutations should be introduced to better enhance the antibody solubility. Here, we perform molecular dynamics simulations combined with the residue-wise decomposition analysis of solvation free energy to address those questions from a solvation thermodynamic viewpoint. We find that, when introducing negatively charged mutations, more favorable solvation is achieved when the mutations are inserted at the site around which more negatively charged residues and fewer positively charged residues are present. Our finding provides a fundamental insight into the location dependence of charged mutations in designing antibodies of enhanced solubility.

Poster Presentation : **PHYS.P-193**
Physical Chemistry
Zoom 4 WED 16:30~17:00

Study on Mechanism of Photo-induced Charge Transfer Using rGO-based Materials as SERS Substrate

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[1]*College of Chemistry, Jilin Normal University, China*

The vibronic coupling enhancement between substrate, molecule, and incident laser, especially the photo-induced charge transfer (PICT) enhancement, is a key to study chemical enhancement of surface-enhance Raman scattering (SERS) mechanism. In this work, through a simple wet chemistry method, two-dimensional SiO_2-Ag-rGO nanosheets were successfully obtained. In this structure, silver nanoparticles (Ag NPs) with uniform size were grown on the surface of graphene oxide, and then the surface modification of reduced graphene oxide (rGO) and Ag NPs was performed using SiO_2. X-ray photoelectron spectroscopy was used to explore the large number of surface defects for rGO nanosheets in SiO_2-Ag-rGO nanosheets. The details of the mechanism of PICT will be discussed in this presentation.

Poster Presentation : **PHYS.P-194**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Poly (acrylic acid) and D-glucosamine-conjugated functionalized gadolinium oxide for highly efficient T_1 magnetic resonance imaging contrast agent

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[1]*Department of chemistry, Kyungpook National University, China*

Magnetic resonance imaging contrast agents (MRI-CAs) distinguish normal and abnormal tissues inside the body through the differential contrast enhancement. For biomedical application MRI-CAs, nanoparticle should be highly water soluble, stable, non-toxic, and ultrasmall in particle size. In This work, we synthesized Gd_2O_3 nanoparticles coated by polyarylic acid (Mw =1800 Da) and D-glucosamine to obtain stable nano colloids, in order to achieve high-performance in vivo T_1 MRI. The ligand was directly coated on the nanoparticle surface with average diameters of ~2nm, which could reduce the toxicity as well as improve the tumor-targeting ability. As the result, the Gd_2O_3 nanoparticles coated with PAA, PAA-1Glucosamine and PAA-2Glucosamine exhibited a high relaxivity as 14.3083 $s^{-1}mM^{-1}$, 13.9348 $s^{-1}mM^{-1}$ and 10.1839 $s^{-1}mM^{-1}$. Afterword, the biocompatibility of these composites was assessed by in-vitro cell viability measurements and in vivo MRI test.

Poster Presentation : **PHYS.P-195**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Ultrasmall gadolinium oxide nanoparticles with cancer targeting ability and its application in *in vivo* neutron capture therapy of cancer.

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Department of Chemistry, Kyungpook National University, Korea

In this work, ultrasmall gadolinium oxides nanoparticles were grafted with polyacrylic acid (PAA) for biocompatibility and colloidal stability, which was then conjugated with cancer-targeting arginylglycylaspartic acid (RGD) (shortly, RGD-PAA-UGNPs). These RGD-PAA-UGNPs were intravenously administered into the tails of nude model mice with cancer. At the time of the maximum accumulation of the RGD-PAA-UGNPs at the cancer site, which was monitored using magnetic resonance imaging, the thermal neutron beam was locally irradiated onto the cancer site and the cancer growth was monitored for 25 days. The cancer growth suppression was observed due to the GdNCT effects of the RGD-PAA-UGNPs, indicating that the surface-modified UGNPs with cancer-targeting ability are potential materials applicable to the in vivo GdNCT of cancer.

Poster Presentation : **PHYS.P-196**

Physical Chemistry

Zoom 4 WED 16:30~17:00

Synthesis, characterization and cellular toxicity of Chitosan Oligosaccharide Lactate-coated Gadolinium Oxide Nanoparticles

Mohammad Yaseen Ahmad, Gang Ho Lee[1,*]

Kyungpook National University, India
[1]*Department of Chemistry, Kyungpook National University, Korea*

Gadolinium oxide nanoparticles (NPs) are considered potential T_1 MRI contrast agents due to high densities of Gd(III) per NP. Therefore, their MRI properties have been extensively studied in vitro and in vivo so far. However, their use as T_1 MRI contrast agents requires suitable surface coating to ensure hydrophilicity and biocompatibility. Surface-coating also provides the NPs with improved relaxometric properties because surface-coating materials can attract water molecules close to a core NP to allow them to have an enhanced interaction. In this study, hydrophilic and biocompatible chitosan oligosaccharide lactate (COL)-coated ultrasmall gadolinium oxide nanoparticles were synthesized. They exhibited very low cellular toxicity and r_1 value of 13.0 $s^{-1}mM^{-1}$ ($r_2/r_1 = 2.1$), which was three times higher than those of commercial magnetic resonance imaging (MRI) contrast agents. The potential of the solution sample as a T_1 MRI contrast agent was confirmed from dose-dependent positive contrast enhancements in R_1 map images.

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Development of Synthetic and Post-synthetic Processes for better Photophysical Properties of Perovskite Quantum dots: Strategies to Improve Photoluminescence Quantum Yield

YeJi Shin, ChaeHyun Lee, Seog Joon Yoon*

Department of Chemistry, Yeungnam University, Korea

Urgently evolved importance to make high quality of raw materials requires researchers to develop creative way to obtain the high quality materials by themselves. Herein, we proposed independent synthetic strategy to achieve key materials with high quality for the perovskite quantum dot research by controlling recrystallization process. Furthermore, to improve Photoluminescence Quantum Yield (PLQY) of the perovskite quantum dots, it is necessary to understand the total charge recombination process to do control systematically. Recently the effort to combine both spectroscopic facilities and facilities for electrochemistry have been raised to elucidate fundamental unknown issues. Thus, we have assembled the two setups to perform *in-situ* spectroelectrochemical characterization, and proposed the way to perform the *in-situ* technique to control the recombination sites. Through two processes - recrystallization and electrodeposition -, we were able to obtain enhanced PLQY by inhibition of recombination sites.

Poster Presentation : **PHYS.P-198**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Alternative Synthetic Strategy of Water Stable Perovskite Quantum Dots in SiOx under ambient condition at room temperature

Soo Jeong Lee, YouJeong Lee, Seog Joon Yoon[1,*]

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

For the next-generation solar cell, the energy payback is also important factor to use the renewable energy, solar light. Silicon-based solar cell has one of critical disadvantage: long-term energy payback time. Fortunately, so far, modern industrial process have reduced its energy payback time to ~ 2 years, but it is necessary to reduce the energy payback time more significantly. However, unfortunately, high-energy required processes are still being used to make photosensitizers for the solar cells, such as II-IV, III-V, I-III-VI semiconductors, quantum dots (QD, synthesized through hot-injection process), polymers, and so on. To reduce the energy payback time significantly, instead of high-temperature and inert gas based synthetic procedure, we propose brand new strategy: perovskite quantum dot synthesis at room temperature in ambient condition. Through in-situ and ex-situ spectroscopic tools, we proposed the formation mechanism of the QDs made through new synthetic process. Furthermore, the intrinsic problem of perovskite – instability against to humidity/water – has been solved by coating silica. We observed the perovskite QDs@SiOx is stable in water during several weeks.

Poster Presentation : **PHYS.P-199**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Ultrasmall Gd_2O_3 nanoparticles surface-coated by three different polyacrylic acids (PAA) and measurement of relaxation properties which

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

Magnetic nanoparticles have great interest due to their potential applications in the field of biomedical theragnosis. Ultrasmall Gd_2O_3 nanoparticles one of the important nanoparticle agents owing to their high content of Gd(III). Which are a prospective positive (T_1) magnetic resonance imaging (MRI) contrast agents. Gd(III) exhibits the highest spin magnetic moment of all elements due to having seven unpaired 4f electrons, that allowing Gd(III) chelates to be clinically administered to patients as T_1 MRI contrast agents. In this study, we characterized PAA-size-dependent relaxometry properties of PAA-coated ultrasmall Gd_2O_3 nanoparticles for three different PAA sizes, were used as ligands, namely PAA1200 (Mw= 1200 Da), PAA5100 (Mw= 5100 Da), and PAA15000 (Mw= 15000 Da), electrostatically binding to Gd(III) at the nanoparticle surface via COOH groups, The R_1 and R_2 values of the obtained composites were measured as a function of PAA size, and the corresponding biocompatibility was investigated in-vitro cell viability tests. Finally, Dose-dependent R_1 MRI map images were recorded to determine the suitability of PAA-coated nanoparticles for use as a potential T_1 MRI contrast agent.

Poster Presentation : **PHYS.P-200**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Carbon coated paramagnetic dysprosium oxide nanoparticles used as a new class of efficient T_2 MRI contrast agent

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Nanoparticles (NPs) are considered as potential candidates for a new class of magnetic resonance imaging contrast agents. And negative MRI contrast agents require high magnetic moments. Whereas, if nanoparticles can exclusively induce the transverse water proton spin relaxation with negligible induction of the longitudinal water proton spin relaxation, they may provide negative contrast MR images even though their magnetic moments are not high, thus acting as an efficient T_2 MRI contrast agent. In this study, carbon-coated paramagnetic dysprosium oxide ($C@Dy_2O_3$) NPs (shell = carbon; core = Dy_2O_3) were synthesized to explore their potential as a T_2 MRI contrast agent at 3.0 T MR field. Due to an appreciable (but not high) magnetic moment of the core Dy_2O_3 NPs which arises from fast 4f-electrons of Dy(III) ($^6H_{15/2}$), the $C@Dy_2O_3$ NPs exhibited an appreciable transverse water proton spin relaxivity (r2) with negligible longitudinal water proton spin relaxivity (r1). Therefore, they acted as a highly efficient T_2 MRI contrast agent and negative contrast enhancements were observed in vivo T_2 MR images.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Room Temperature Quantum Dot Synthesis and its Optimization Process: Formation Mechanism Observed through in-situ Spectroelectrochemical Setup

YouJeong Lee, Soo Jeong Lee, Seog Joon Yoon[1,*]

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

Recent energy demands for human being have raised exponentially. The researches to develop and to utilize the alternative energy resources have contributed to retard the global warming. One of promising renewable energy, solar energy, have been utilized through silicon-based solar cells, which are available in commercial market. However, even though the significant mass production of the Si-solar cells from China have contributed to reduce the energy payback time, however, the Si-solar cell still requires the energy payback time about 2 years. This is because one of the fabrication processes requires the high energy input to melt silicon and generate polycrystalline Si wafer. Compared to the high energy input process, we demonstrated room-temperature inorganic photosensitizer synthetic procedure. Fabrication of perovskite quantum dots (PQDs) under ambient condition at room temperature could significantly reduce the energy payback time. We optimized the fabrication process and we were able to observe the PQD@SiOx. Through in-situ spectroelectrochemical setup, we were able to clarify the formation mechanism of PQD@SiOx.

Poster Presentation : **PHYS.P-202**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Temperature effect on size-controlled one-pot synthesis of poly (acrylic acid-co-maleic acid) coated platinum oxide nanoparticles as a CT contrast agent

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

Poly (acrylic acid-co-maleic acid) coated platinum oxide nanoparticle for the first time through a simple one-pot polyol synthesis as a CT Contrast agent. In this work, the particle size was controlled by modifying the temperature so that the particle size decrease by increasing temperature. Two particle diameters were prepared at two different temperatures with an average size of 4.23 nm (T= 110oC) and 2.2 nm (T= 250oC). Nanoparticles were characterized by XRD, TGA, FTIR, TEM, and also X-ray absorption intensity of nanoparticles studied and was stronger than those of commercial molecular iodine CT contrast agent at the same atomic concentration and much stronger at the same number density. This finding proved the potential of platinum oxide nanoparticles as a high- performance CT imaging.

Poster Presentation : **PHYS.P-203**

Physical Chemistry

Zoom 4 WED 17:00~17:30

A simulation study on the spatial arrangement and the dynamics of a ring polymer chain in thin linear polymer films

Jong Ho Choi, Bong June Sung*

Department of Chemistry, Sogang University, Korea

A ring polymer chain is topologically different from a linear polymer chain: there is no chain end in the ring chain. The ring chain is, therefore, subject to small conformational fluctuations and hardly entangle other ring chains, thus being easily processable polymeric materials with low viscosity. When the ring chain is mixed with linear chains, the ring chain diffusion may be complicated because the linear chain may penetrate through the ring chain and hinder its diffusion. A recent study showed that ring chains were not uniformly distributed in polymer films of ring and linear polymer mixtures(Phys. Rev. Lett. 118, 167801 (2017)). Since the local viscosity of polymer films is spatially heterogeneous and the local viscosity of the interfacial region is usually lower than that of central regions, such a non-uniform distribution of ring polymer chains may lead to heterogeneous ring diffusion. In this work, we perform molecular dynamics simulations for the thin polymer films of a single ring polymer chain and linear polymers in order to investigate the ring chain diffusion. We find that the ring chain is located mostly in the central (interfacial) regions when the interaction between monomers of the ring and the linear chain is slightly more (less) attractive. This suggests that the spatial arrangement of the ring chain in films should be an energetically driven process. When the ring chain is preferentially in the interfacial (central) regions, the ring chain diffuses faster (slower). Therefore, the ring chain diffuses two different diffusion coefficients within the film, thus leading to spatially heterogeneous and non-Gaussian diffusion, and reflecting the local viscosities of the films faithfully.

Poster Presentation : **PHYS.P-204**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Study of Thermoresponse of Odd-Even Effect in n-Alkanethiolate Self-Assembled Monolayers

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Department of Chemistry, Korea University, Korea

Recently, understanding of how thermal heating affects chemical and physical properties of individual molecules, particularly structurally simple alkane(di)thiols, has received significant attention. This presentation shows a study of thermoresponse of supramolecular packing structure of self-assembled monolayers of n-alkanethiolates (SCn, n = 3 – 18) formed on ultraflat template-stripped gold (Au^{TS}). In particular, focus is placed on answering the question: does thermal heating affect the odd-even effect in SCn SAM? What is that origin? Interestingly, and unexpectedly, experiments using sum frequency generation spectroscopy (SFG) revealed that thermoresponse of SFG signal remarkably depended on the length of n-alkane chain. As the heating temperature increased, i) short SAMs (n = 3 – 9) exhibited decreased SFG signals for both asymmetric and symmetric C-H stretching of terminal CH_3, ii) for long SAMs (n = 10 – 18), one of the stretching modes decreased symmetric and asymmetric stretching modes for the even and odd, respectively, and iii) The terminal ethyl groups rotate in the same direction for even and odd cases. This rotational motion induces a different variation of the tilt angle of terminal methyl ($\Delta\theta$) for the odd and even because the direction of the terminal ethyl was different at room temperature each other. Therefore, the thermoresponse of tilt angle of terminal CH_3 (θ) relative to the surface normal for odd and even SAMs was opposite. These SFG findings were further reconciled with results of water droplet contact angle measurements. Finally, we can explain how heat-induced structural changes depend on the chain length of the SCn based on SFG and contact angle results.

Poster Presentation : **PHYS.P-205**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Optical Kerr effect in Liquid Visualized by Femtosecond X-ray Solution Scattering

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

We studied the molecular dynamics in a dye solution using femtosecond time-resolved x-ray solution scattering (fs-TRXSS) techniques. The variation of the scattering signal we measured was consistent with the optical Kerr effect (OKE) phenomenon. This is because the signals obtained from the fs-TRXSS have a different form than the solvent-heating signals already well known in previous studies. Thus we compared and analyzed the scattering data with molecular dynamic simulation studies, and were able to simulate this as a change in the arrangement between solute and solvent molecules. The simulated scattering signal well reproduces the measured time-resolved scattering signal.

Poster Presentation : **PHYS.P-206**
Physical Chemistry
Zoom 4 WED 17:00~17:30

A Simulation Study on the breakdown of time-temperature superposition principle for Poly(ethylene oxide) melts

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The elastic moduli of linear viscoelastic materials at a wide range of temperatures can be estimated by superimposing the elastic moduli of different time scales at a reference temperature. This is known as the time-temperature superposition (TTS) principle and has been employed extensively in industry to develop various viscoelastic materials. TTS is based on the assumption that the relaxation time (or the friction constant, ζ_i) of all modes of polymers would have the same temperature dependence. Unfortunately, TTS sometimes breaks down, especially close to the glass transition, of which origin remains a matter of debate. We elucidate whether the breakdown relates to the spatial heterogeneous dynamics. We employ OPLS-AA force field and perform all-atom molecular dynamics simulations for poly(ethylene oxide) (PEO). Understanding the mechanical properties of PEO has been an importance topic due to the usage of PEO as the next generation solid polymer electrolytes. We calculate the dynamic structure factor F_i (k,t) (which is the Fourier-transform of the space-time correlation function of a polymer segment) for several segmental modes of PEOs. Here, *i, k,* and *t* denote the index of each segmental mode, a wave vector and time, respectively. We, then, estimate the friction coefficient ζ_i of the ith segmental mode by fitting F_i (k,t) to a Kohlrausch-Williams-Watts (KWW) stretched exponential function. We find that as temperature decreases down to the glass transition temperature, the segmental dynamics becomes heterogeneous such that the ratios of ζ_i's decouple to one another and ζ_i's do not show identical temperature dependence, which is against the underlying assumption and breaks down the TTS.

Poster Presentation : **PHYS.P-207**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Advanced Synthetic Method of Organic Inorganic Hybrid Material using Pulsed Laser Ablation in Liquid

Juhyeon Park, Yiseul Yu, Shreyanka Shankar Naik, Yujeong Jeong, Tae Ho Kim*, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Herein, we have successfully synthesized organic-inorganic hybrid materials (OIHM) using pulsed laser ablation (PLA) in liquid medium. Firstly, the N-type organic ligand (**L**) having a charge-transfer characteristic was synthesized by reaction of 3-(methylthio)propylamine and pyromellitic dianhydride. Further, OIHM was prepared by using PLA technique. Where interaction of copper target with focused Nd:YAG laser (λ=532nm) generates copper ions and electrons. In addition, the acetonitrile molecules present in close proximity of the target dissociate to form CN^- . These Cu ions interact with CN^- and **L** leading to the formation of OIHM. Single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after PLA. OIHM was crystallized in space group Triclinic P-*1*. The $[CuCN]_n$ chain, which is the central axis in the structure is interconnected by **L**s to form a linear 1D line, which is infinitely connected. This chain is combined with **L** to have a 3D network structure. This study delivers an one pot synthesis of OIHM using eco-friendly, facile and rapid technique of PLA. Also, the mechanism of formation, structure, thermal, and electrical properties of the new copper centered OIHM using PLA was illustrated. We hope this approach is a novel and a significant method for the synthesis of organic-inorganic hybrid materials.

Poster Presentation : **PHYS.P-208**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Tracers dynamics reveals the local media structure and diffusion mechanism of two-dimensional polydisperse colloidal glasses

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When glass-forming liquids cool down to glass transition temperature, its dynamics not only drastically slows down but also becomes highly heterogeneous. Even though glasses are ubiquitous in our daily life, it remains an unsolved problem whether the glass transition would be a kinetic trap or a thermodynamic phase transition. In addition, the presence of the structural order in glass-forming liquids has been a topic of study for decades. It is, however, a non-trivial task to identify and analyze the structural order in glass-forming liquids. We suggest an in-direct way of scrutinizing the local structural order by introducing tracers as stand-ins. We perform molecular dynamics simulations for two-dimensional (2D) polydisperse colloids with tracers. 2D polydisperse colloids are well-known to exhibit local structural orders depending on the polydispersity of their size distribution. When the polydispersity is small around 0, colloids are almost monodisperse and develop hexatic structures. As the polydispersity increases, hexatic structures become less prominent. We employ two different types of tracers: diamond tracers and square tracers. Diamond tracers are commensurate with hexatic structures of monodisperse colloids while squares are not. When the polydispersity is low, the rotational diffusion of square tracers is much more enhanced than that of diamond tracers because diamond tracers have to break the structural commensurateness and overcome a larger free energy barrier. When the polydispersity increases, the difference in diffusion between diamond and square tracers dies away. Our simulation results illustrate that the tracer diffusion can reflect the local hexatic structures of glasses and can be used to investigate the structural order.

Poster Presentation : **PHYS.P-209**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Study of Non-polar Additive Effect to Solvation Structure in Lithium-Ion Battery Electrolytes by FTIR Spectroscopy

Joo Hyun Kim, Chaiho Lim, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

Lithium-Ion batteries are highly demanding battery among other rechargeable batteries due to its high-voltage window and energy density. In the development of lithium-ion batteries, it is important to develop appropriate electrolytes because the electrolyte is a charge carrier in lithium-ion rechargeable battery between anode and cathode material which crucially affects the conductivity of batteries. To understand and enhance the properties of electrolytes, it is important to understand the solvation nature of lithium ion in the electrolytes. Recently, a new method IR-DOSY (Internally Referenced DOSY-NMR) has been reported to study the solvation structure in binary systems that are usually complicated to study in vibrational spectroscopy. IR-DOSY technique adds a small amount of toluene inside the electrolytes and uses the toluene as an internal reference to calculate the solvation ratio of lithium ions in the electrolyte since toluene does not participate in the first solvation shell. However, we found the addition of toluene affects the solvation nature of lithium ion in the electrolytes. In other words, the addition of toluene did not avoid the perturbation of the first solvation shell compared to toluene not added electrolytes. In this study, we represent the effect of toluene to the solvation nature in electrolytes by Fourier-transform infrared spectroscopy (FTIR).

Poster Presentation : **PHYS.P-210**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Comparison of segmental dynamics of polymer-tethered probes in a single component system and free probes in miscible blends

Hyangseok Lee, Keewook Paeng*

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The segmental dynamics of polymers are measured by monitoring fluorescent probes in host polymer matrices via rotational fluorescence correlation microscopy. By changing the number of tethering points of probes to the polymer, we were able to control local concentration of polymer near the fluorescent molecule. Dynamics of free probes in a binary mixture are compared with that of tethered probes in a single component system. The rotational dynamics of tethered probes were slower than the freely rotating probes due to the restricted motion by tethering, but the temperature dependence of polymer dynamics matched with that of the hosts. On the other hand, the β value which is the measure of dynamic heterogeneity in the system, was lower than that of host and similar to that of tethered polymer. In case of free probes in binary blends, the temperature dependence and the β value were similar to the analysis of tethered polymer except showing double decay in autocorrelation functions.

Poster Presentation : **PHYS.P-211**

Physical Chemistry

Zoom 4 WED 17:00~17:30

The effects of the phase separation and the local domains of ternary mixture lipid bilayers on the diffusion of cholesterol

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The diffusion of cholesterol in biological membranes is critical to cellular processes such as the formation of cholesterol-enriched domains. According to a recent study (*J. Phys. Chem. Lett. 2018, 9, 6529-6535*), the cholesterol undergoes flip-flops between leaflets of DPPC lipid bilayers and exhibits anomalous non-Gaussian diffusion. The flip-flop, a dominant transport mechanism for cholesterol, is also known to depend on the lipid types of the bilayers. Since cell membranes consist of various types of lipids and form domains, the diffusion and the flip-flop of cholesterol should be complicated. In order to investigate the effects of domains on the cholesterol transport, we perform molecular dynamics simulations up to 50 μsec for ternary systems of saturated lipids (DPPC), unsaturated lipids (DIPC) and cholesterol. We change the fraction (X_{chol}) of cholesterol from 0.1 to 0.3. We observe that DPPC-rich domains and DIPC-rich domains appear after 1.5μsec regardless of X_{chol} and that cholesterol prefers DPPC-rich domains. We find that cholesterol can flip-flop within both DPPC-rich and DIPC-rich domains. However, cholesterol in DPPC-rich domains has to overcome a larger free energy barrier to perform flip-flops than in DIPC-rich domains. More interestingly, cholesterol in DPPC-rich phases becomes more meta-stable at the central region in between two leaflets while cholesterol in DIPC-rich phases is unstable at the central region. This suggests that even though it should take more time for cholesterol in DPPC-rich domains to flip-flop than in DIPC-rich domains, the cholesterol may stay for a longer time in the central region, thus its diffusion becoming more heterogeneous.

Poster Presentation : **PHYS.P-212**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Debye-Stokes-Einstein equation breakdown in the polymer system via fluorescence correlation microscopy.

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The segmental dynamics of polymer can be probed by analyzing fluorescent molecules in polymer matrices via fluorescence correlation microscopy (FCM) which can determine both translational and rotational diffusions in the polymer system depending on the frame rate of the measurements. In this study, we measured the translational and rotational motions of p-Phenylenediamine (pPDI) in polystyrene as function of temperature down to the glass transition temperature (Tg). Upon cooling the sample from the temperature far above Tg, Debye-Stokes-Einstein relationship which successfully describes the rotational and translational motions in normal liquids has breakdown starting from 1.2 Tg ,and the magnitude of breakdown increases as much as approximately 4.8 decades at Tg.

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Evaluation of Photocatalytic Activity of ZnO/Au/g-C_3N_4 Ternary Nanocomposite under Simulated Solar Light Irradiation

Talshyn Begildayeva, Seung Jun Lee, Yiseul Yu, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Ternary nanocomposite ZnO/Au/graphitic carbon nitride (g-C_3N_4) was fabricated via a facile and eco-friendly pulsed laser ablation (PLA) and pulsed laser irradiation (PLI) methods without any capping agents or surfactants. The as-prepared photocatalyst was characterized by various electron microscopy and spectroscopy techniques, which prove the good dispersion of the Au nanoparticles (NPs) on the surface of spherical ZnO particles deposited on the g-C_3N_4 nanosheets. Ternary nanocomposite showed photocatalytic activity in degradation of methylene blue (MB) dye under simulated solar light illumination. In particular, various amount of gold doped onto bare ZnO and different weight percent (wt%) of g-C_3N_4 in the composite were tested. For instance, ZnO/Au15/g-C_3N_4 containing 15 wt% Au displayed a rate constant, which is 3 and 5 times greater than those of bare g-C_3N_4 and ZnO, respectively. This improved photocatalytic activity of nanocomposite is due to the surface plasmon resonance of Au NPs and the synergistic effects between ZnO and g-C_3N_4. There is in this nanocomposite direct migration of the photogenerated electrons from g-C_3N_4 to ZnO/Au, which hinders the recombination of electron–hole pairs and enhances the charge separation efficiency. In addition to the experimental studies, a plausible MB degradation mechanism over the ZnO/Au/g-C_3N_4 photocatalyst is proposed based on the results of the scavenger study.

Poster Presentation : **PHYS.P-214**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Spectroscopic study of ceria NPs for radical quencher in fuel cell

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The purpose of this study is to confirm the ability of radical quencher by the spectroscopic study. Polymer electrolyte membrane fuel cell (PEMFC) has many advantages such as compact construction, high efficiency and low working temperature. But when the fuel cell operates, hydroxyl radicals generated and will decrease the efficiency of the fuel cell. If the hydroxyl radicals can be reduced, the fuel cell's ability will improve. There are some radical scavengers such as cerium ion, cerium oxide, transition metal, and polymer having redox properties and we used cerium oxide as the radical scavenger.Therefore, in this study, ceria NPs doped with three different materials such as ceria@TTAB, ceria@DSA and ceria@Dmp were prepared to confirm the ability of these radical scavengers. To examine the radical quenching activity of various forms of cerium oxides, we used a fluorescent dye, 6-carboxylfluorescein (6-CFL), as a probe. 6-CFL degrades in the presence of hydroxyl radicals, resulting in the decrease of the intensity of its photoluminescence (PL). Time-dependent PL intensity were measured various forms of cerium oxides using a fluorescence spectrometer. Then temporal decay of PL intensity was calculated from fitting with a single exponential function for results analysis.As a result, PL decay becomes slower in the order of ceria@TTAB, ceria@DmP. PL measurements demonstrate the radical quenching ability of ceria NPs increase in the order of ceria@TTAB < ceria@DmP < ceria@DSA.It was confirmed that ceria@DSA has a good radical quenching ability, and it can improve the efficiency of the fuel cell.

126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **PHYS.P-215**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Orbital asymmetry in electron attachment to trihalobenzene molecules

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Electron attachment to tri-halobenzene molecules were studied using Gaussian package. Calculations were performed using hybrid DFT such as B3LYP, O3LYP, and B3P86. For the molecules containing I, 1, 3-diiodo-2-chlorobenzene (DICB) and 1, 3-diido-2-bromobenzene (DIBB), effective core potential (ECP) was considered. When an electron was added to the tri-halobenzene, negative charges were expected to be distributed in the order of Cl>Br>I, but opposite results were obtained according to orbital asymmetry. Adiabatic electron affinity (AEA) and vertical detachment energy (VDE) were obtained and compared. Differences in these values were observed depending on the basis sets used, but the VDE-AEA value were similar to each other.

Poster Presentation : **PHYS.P-216**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Ultrafast Charge Transfer Dynamics of Silver Bismuth Iodide by using Time-Resolved spectroscopy

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In the previous study about solar cells, many researchers had studied Pb-based $CH_3NH_3PbX_3$ ($MAPbX_3$) perovskite solar cells. Because it has advantages such as high photovoltaic conversion efficiency (PCE, >20%), facile fabrication process, low cost, easily tunable bandgap, etc. But Pb-based solar cells cause environmental problems and have poor stability. In this research, we synthesized Bi-based material, silver bismuth iodide (SBI). SBI is eco-friendly and more stable than Pb-based perovskite solar cells. However, the PCE of SBI is much lower than 2 %. To improve the PCE, we used copper as a dopant. To analyze the charge transfer dynamics of SBI (FTO/TiO_2/SBI) and Cu:SBI (FTO/TiO_2/Cu:SBI), we used spectroscopic methods such as UV-Vis and transient absorption spectroscopy (TAS).). In the UV-Vis spectra of SBI and Cu:SBI synthesized in various copper ratio. When Cu doped, the absorption coefficient increased and Cu:SBI absorbs about 30 % more photons than SBI. The higher absorption coefficient means that the devices can generate more charge carriers. And through the tauc-plot , the bandgap is 1.82 eV for SBI. We used TAS to investigate charge carrier dynamics of the SBI and Cu:SBI with photoexcitation 355 nm by using nanosecond transient absorption spectrometer. The decays of each TA signal at 650 nm and their fitting parameters are obtained with single exponential fitting. The time constants (τ) of SBI and Cu:SBI are 488.9 and 413.4 ns and amplitudes (A) are 2.739 and 0.904, respectively.

Poster Presentation : **PHYS.P-217**
Physical Chemistry
Zoom 4 WED 17:00~17:30

Role of cyclopentadienyl ligands of group 4 precursors toward high-temperature atomic layer deposition

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Deposition of high-k dielectric thin films is crucial in the fabrication of modern electronic devices. Atomic layer deposition (ALD) is one of the most attractive technology for depositing high-k materials owning to conformality and thickness control of the films at the atomic level. It has been suggested that high-temperature ALD can enhance the material properties of the films such as density and crystallinity, for which development of thermally stable precursors that deliver the metallic element is required. Recently, heteroleptic Zr and Hf precursors containing amido and cyclopentadienyl (Cp) ligands are introduced, some of which show enhanced thermal stability. However, the mechanism behind the enhanced stability of these precursors remain unclear. In this study, we aim to suggest theoretical design rules for the chemical structure of group 4 (Ti, Zr, Hf) precursors toward high-temperature ALD via density functional theory (DFT) calculations. First, the gas-phase decomposition of group 4 precursors are considered. By observing several pathway, β-H elimination between amido groups are found to be the preferred decomposition path for the considered precursors. Second, surface reactions of the precursors on oxide surfaces are considered. For most precursors, one or two of the ligands are suggested to remain upon chemical adsorption. Especially, the Cp ligands are suggested to persist on the surface, while amino ligands are easier to be removed during adsorption. Then, decomposition of the precursor after adsorption on the surface is considered, for which Cp is shown to significantly increase the thermal stability. Our result intends to offer a fundamental molecular-level understanding of the thermal stability of group 4 precursors for high temperature ALD.

Poster Presentation : **PHYS.P-218**

Physical Chemistry

Zoom 4 WED 17:00~17:30

Laser assisted synthesis of reduced graphene oxide (rGO) supported ZnO/Au nanostructures in liquid with enhanced solar light photocatalytic activity.

Shreyanka Shankar Naik, Seung Jun Lee[1], Talshyn Begildayeva[1], Yiseul Yu[1], Hyeyeon Lee[1], Myong Yong Choi[1,*]

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In the present study, solar light active ZnO/Au/rGO ternary nanocomposites were successfully synthesized using Pulsed Laser Ablation (PLA) technique in liquid medium without the aid of surfactant or binders. The crystalline structure, surface morphology, size distribution, elemental composition, and optical properties of the prepared ZnO/Au/rGO ternary nanocomposites were characterized using X-ray diffraction, field-emission scanning electron microscope, high-resolution transmission electron microscope, energy-dispersive X-ray spectroscopy, UV–vis diffuse reflectance spectra, and photoluminescence analysis. The density of the elemental and carbonaceous components like Au nanoparticle and rGO nano-matrix on ZnO could be altered by changing the concentration of HAuCl4.3H2O (5% 10%, 15% and 20%wt) and rGO as (2.5%,5%,7.5%wt) using laser irradiation and wet impregnation technique. The photocatalytic activity of as synthesized nanocomposites were evaluated for the degradation of Methylene Blue (MB) under solar light irradiation. The selective ratio of components in ZnO/Au15/rGO5 exhibit 3 times faster photodegradation kinetic efficiency than bare ZnO. The enhanced photocatalytic activity is attributed to the efficient separation and transfer of photo induced electron-hole pairs (e--h+) in ZnO/Au15/rGO5 ternary nanocomposites. The superior photocatalytic activity revealed that Au and rGO are well anchored onto the ZnO. So, ZnO/Au15/rGO5 ternary nanocomposites could be an exceptionally promising material for waste water treatment and other environmental remediation applications.

Poster Presentation : **PHYS.P-219**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Edges Controlled Oxidation of Two-Dimensional Transition Metal dichalcogenides

Myeong in Song, Sunmin Ryu*

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In-plane anisotropy in various material properties of two-dimensional (2D) crystals is not only intriguing but also of potential use for many applications. In this work, we studied how the structural anisotropy influences oxidation of 2D semiconducting transition metal dichalcogenides (TMDs) in the form of MX_2, where M = Mo and W; X = S and Se. Single and few-layer TMD samples mechanically exfoliated on varying kinds of substrates were characterized for thickness by their differential reflectance and atomic force microscopy (AFM) topography image, and thermally oxidized in controlled Ar: O_2 gas mixture at elevated temperatures of 280 ~ 380 ºC. Oxidation was initiated from randomly distributed reaction centers and led to triangular oxides (TOs) and triangular etch pits (TEs) of varying roundness that were revealed by AFM phase and topography images, respectively. To quantify the roundness of a given triangular object, we defined an isotropy index, R, a size ratio between its inscribed circle and circumcircle. TOs of WX_2 showed larger isotropy values than TEs in MoX_2, indicating that more anisotropic oxidation reactions occur in the latter. The reaction rates of edges increased in the order of M-zigzag, armchair, and X-zigzag, but degree was different in MoX_2 and WX_2, which is consistent with the TEs and TOs. In addition, the typical densities of TOs and TEs were 10 times higher in MSe_2 than MS_2, which suggests that the former contains more reaction centers, possibly structural defects. Finally, $MoSe_2$ and WS_2 showed the lowest and highest reaction barriers, respectively.

Poster Presentation : **PHYS.P-220**
Physical Chemistry
Zoom 4 WED 17:30~18:00

Pulse- and Potentiostatic-Electrodeposition of Cu on Carbon Paper Electrode for Electrochemical Reduction of CO_2

Sena Lee, Min Young Cho, Do Yun Park, Kuan Soo Shin*

Department of Chemistry, Soongsil University, Korea

Carbon dioxide (CO_2) is one of the main gases produced by human activity and is responsible for the greenhouse effect. Numerous pathways for CO_2 capture and reduction are currently under investigation. One approach to reducing the amount of CO_2 is an electrochemical method that converts CO_2 into useful chemicals and fuels. Among the metal electrocatalysts, copper is a unique metal catalyst that can reduce CO_2 to valuable hydrocarbons and oxygenates, such as ethylene, carbon monoxide, and formate. In this work, copper (Cu) nanocomposite has been coated on carbon paper (CP) via pulse electrodeposition (Pul-ED) and potentiostatic electrodeposition (Pot-ED) methods. The Pul-ED and Pot-ED characteristics of Cu deposition on CP (Cu-CP) electrodes were investigated by using scanning electron microscopy, X-ray photoelectron spectroscopy, and powder X-ray diffraction. The gaseous products were analyzed using a gas chromatograph. The remarkable differences between Pul-ED Cu-CP and Pot-ED Cu-CP electrodes in composition, catalytic activity, and Faradaic efficiency for the electrochemical reduction of CO_2 have been found and will be discussed.

Poster Presentation : **PHYS.P-221**
Physical Chemistry
Zoom 4 WED 17:30~18:00

Enhancement of structural stability of electron transport layer in OLED by mixing n-type dopant material.

Minseok Ki, Keewook Paeng[*]

Department of Chemistry, Sungkyunkwan University, Korea

4,7-Diphenyl-1,10-phenanthroline (Bphen) is widely used as electron transport layer (ETL) in organic light emitting diodes (OLED) and has advantages of high electron mobility and the conductivity. However pristine Bphen has structural instability due to its low glass transition temperature (T_g, T_g= 335 K) and fast crystallization at the vacuum and ambient conditions which shortens the lifetime of the device. By mixing an n-type dopant material, 8-hydroxyquinolinolato-lithium (Liq) with Bphen, the crystallization of ETL can be inhibited along with increase in the T_g. It is observed that 5 and 10 vol% mixing of Liq can inhibit crystallization at vacuum and ambient conditions, respectively along with increase in the T_g according to the amount of higher T_g component Liq (T_g= 370 K) doped, roughly following Gibbs-Dimarzio mixing rule.

Poster Presentation : **PHYS.P-222**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Fabrication of metal and metal oxide nanowires using anodic aluminum oxide templatesSher Ali Khan, Chang Min Kim.Department of chemistry, Kyungpook National University.

Sher Ali Khan

Chemistry, Student /Research assistant, Korea

Abstract:Nano wires have wide variety of applications in modern technology and researches like catalysis, electronic devices, gas sensors, energy storage materials and devices with new properties. Anodized aluminum oxide (AAO) template can be utilize to fabricate nanowires. AAO templates with various pore size have been produced by changing factors such as temperature, second anodization time and electrolyte concentrations. Nanowires of different metals have been fabricated inside the pores of template by direct electrochemical deposition using Metal containing electrolytes. Their properties were analyzed by Atomic Force Microscopy (AFM) and Field Emission Scanning Electron Microscopy (FE-SEM).We will report the synthesis of Ni, Zn and ZnO nanowires of various diameters.

Poster Presentation : **PHYS.P-223**
Physical Chemistry
Zoom 4 WED 17:30~18:00

Translational and Rotational Dynamic Heterogeneity induced by Vacancies in Organic Ionic Plastic Crystals

Hyungshick Park, Bong June Sung[*]

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystals (OIPCs) are crystals of electrolytes with a long-range translational order. However, some rotational modes of ions in OIPCs are activated even in solid phases such that the diffusion of dopants may be facilitated. Therefore, OIPCs have been investigated as good candidates for solid electrolytes. A recent NMR experiment observed heterogeneous ion diffusion in the presence of defects: some ions diffused fast while other ions diffused slow (J. Phys. Chem. C 117, 5532 (2013)). Previous simulation studies illustrated that the rotational diffusion should be also heterogeneous (J. Phys. Chem. B 124, 6894 (2020)). Fast ions undergo either rotational or translational hopping motions such that they can diffuse much faster than expected from the solid viscosity. Therefore, the dynamic heterogeneity would be a transport mechanism for the facilitated ion diffusion of the solid electrolytes. In order to investigate the effects of defects on the dynamic heterogeneity of OIPCs, we perform atomistic molecular dynamics simulation of 1,3-dimethylimidazolium hexafluorophosphate ([MMIM][PF_6]) with 1 pair of a cation vacancy and an anion vacancy. At low temperature, vacancies undergo hopping motions toward each other and form a charge-neutral cluster. At high temperature, two vacancies diffuse via hopping and act like a loosely bonded molecule with two vacancies kept close to each other. Translational diffusion of ions is correlated strongly with the vacancy diffusion and becomes heterogeneous when vacancies hop. Rotational motion of ions is also activated when the ions are close to vacancies. Interestingly, the rotational motions are more activated when two vacancies are separated each other even though bound vacancies create a larger free volume.

Poster Presentation : **PHYS.P-224**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Fabrication of metal and metal oxide nanowires using anodic aluminum oxide templates

Sher Ali Khan, Chang Min Kim[1,*]

Chemistry, Student /Research assistant, Korea
[1]*Department of Chemistry, Kyungpook National University, Korea*

Nano wires have wide variety of applications in modern technology and researches like catalysis, electronic devices, gas sensors, energy storage materials and devices with new properties. Anodized aluminum oxide (AAO) template can be utilize to fabricate nanowires. AAO templates with various pore size have been produced by changing factors such as temperature, second anodization time and electrolyte concentrations. Nanowires of different metals have been fabricated inside the pores of template by direct electrochemical deposition using Metal containing electrolytes. Their properties were analyzed by Atomic Force Microscopy (AFM) and Field Emission Scanning Electron Microscopy (FE-SEM).We will report the synthesis of Ni, Zn and ZnO nanowires of various diameters

Poster Presentation : **PHYS.P-225**
Physical Chemistry
Zoom 4 WED 17:30~18:00

NiPd alloy electrocatalysts synthesized by Pulsed Laser irradiation in liquid phase

Yiseul Yu, Theerthagiri Jayaraman, Seung Jun Lee, Shreyanka Shankar Naik, Myong Yong Choi*

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The development of electrocatalytically active materials has attracted much attention due to their broad range of potential applications. In this study, we proposed a new advanced integrated technology of pulsed laser and ultrasonic chemical processes for the production of metals, alloys and composites. Nickel palladium alloy structures were prepared by two step process. Initially, Ni particles was produced by pulsed laser ablation of Ni metal plates in methanol. Then, the prepared Ni particles was added to the palladium salt solution and irradiated with unfosed laser under ultrasonic waves to produce NiPd alloy. The structural and morphological properties of the NiPd alloys were characterized by various analytical techniques viz., X-ray diffraction (XRD), field emission scanning electronic microscope (FE-SEM). Energy dispersive X-ray spectroscopy (EDS) and dynamic light scattering (DLS). Finally, the synthesized NiPd alloy was applied as an electrocatalyst for the hydrogen evolution reaction (HER).

Poster Presentation : **PHYS.P-226**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Understanding Dynamic Heterogeneity using tethered probes by isolating temporal heterogeneity from spatial heterogeneity

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Tethered probes could provide a deeper understanding of glass dynamics near glass transition by isolating rotational motion from that of translation. In previous studies, freely rotating probes are used to study dynamic heterogeneity by measuring median β as a function of trajectory length, however this results cannot distinguish spatial heterogeneity and temporal heterogeneity. Therefore, we used tethered probes to observe only temporal heterogeneity by restricting translational motion. The median β as a function of trajectory length of tethered probes are converged slower than that of freely rotating probes. Also, we found that the rotational dynamics of tethered probes was found to be slower than freely rotating probes, but the temperature dependence of polymer dynamics and the distribution of rotational dynamics of tethered probes were not changed.

Poster Presentation : **PHYS.P-227**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Computational Study on the Structural and Thermodynamic Features of SOD1

Haeri Im, Sihyun Ham*

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Amyotrophic lateral sclerosis (ALS) is a selective dying disease of the spinal motor nerves. Although it is a progressive incurable disease, there is no proper treatment currently available. Excessive SOD1 and its mutants undergo protein aggregations in neurons, which are supposed to spread to adjacent cells, leading to the death of nerve cells. Therefore, the mutation of the SOD1 induces genetic ALS, and it is presumed that it plays a role in the sporadic type of non-genetic ALS disease. In this study, we investigate the effect of individual mutations on the structural and thermodynamic properties of the SOD1. We perform molecular dynamics simulations to probe structural changes induced by the mutations, and then carry out solvation free energy calculations to analyze thermodynamic features. Our study will contribute to an understanding of the SOD1 aggregation associated with ALS disease, and also provide the structural basis for developing drugs that inhibit the aggregation.

Poster Presentation : **PHYS.P-228**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Synthesis of Au-Pd alloy using pulsed Laser irradiation in liquid phase and their catalytic performance

<u>Kim Jiwon</u>, Yiseul Yu, Seung Jun Lee[1], Theerthagiri Jayaraman[1], Myong Yong Choi[1,*]

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Bimetallic Au-Pd alloys exhibits unique physicochemical and catalytic properties which are mainly dependent on their surface morphology and chemical composition. Herein, we synthesized Au-Pd alloys by pulsed laser ablation (PLA) of a metal salts in aqueous media without using of any reducing agent. The structural and morphological analysis was examined by various analytical techniques such as, X-ray diffraction (XRD), UV-visible absorption (UV-Vis), field emission scanning electron microscope (FE-SEM), and energy dispersive X-ray spectroscopy (EDS). The synthesized Au-Pd alloys can efficiently use for catalytic applications. Apart from the shape and size, tailoring of chemical composition is also another efficient way to tune the catalytic performance.

Poster Presentation : **PHYS.P-229**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Facile synthesis and characterization of Nitrogen doped ZnO for the efficient photocatalytic degradation of Tetracycline under Visible light.

Sang Hun Yeon, Shreyanka Shankar Naik[1], Seung Jun Lee[2], Theerthagiri Jayaraman[2], Myong Yong Choi[2,*]

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Abstract: Zinc oxide (ZnO) is considered as a potential material among metal oxide semiconductors. However, the setbacks of the ZnO can be corrected using non-metal doping on ZnO. Nitrogen is considered as a promising candidate for doping because of similar atomic radius and lower ionization energy and electronegativity creates a shallow acceptor level in ZnO. Herein, we have successfully synthesized Nitrogen doped ZnO (ZnO: N) using pulsed laser assisted technique in various concentration of urea solution. The synthesized material were characterized using HR-TEM, FE-SEM, XRD, UV-Visible, Micro-Raman and Photoluminescence spectra. As prepared material treated for the degradation of tetracycline under visible light illumination (VLI). The photocatalytic activity (PCA) of ZnO: N performed on an antibiotic tetracycline pollutant .The ZnO: N nanomaterial showed higher degradation of TC than pristine ZnO. Hence, Nitrogen doping helps in changing intrinsic characteristics of the material. The excited electron is trapped in the accepter level of nitrogen. Hence; induced charges are separated and helps in generation of reactive oxygen species (ROS). The ZnO: N nanomaterial has same potential applications as of ZnO. Our work provides a rational design of photocatalyst for environmental remediation.

Poster Presentation : **PHYS.P-230**

Physical Chemistry

Zoom 4 WED 17:30~18:00

SERS-sensitive Gold Nanoparticles Synthesized by Pulsed Laser Ablation in acetonitrile and water mixtures

Hyeyeon Lee, Talshyn Begildayeva, Seung Jun Lee, Seung Heon Lee, Young Wook Lee[1,*], Myong Yong Choi[*]

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Herein the laser-assisted synthesis of gold nanoparticles (Au NPs) in the mixture of acetonitrile and water is reported. A volume ratio of acetonitrile in the reaction mixture used as liquid media during pulsed laser ablation (PLA) method can affect on the final properties of Au NPs. By varying acetonitrile volume percent in the mixture with water, the size of Au NPs and the thickness of graphitic carbon (GC) shells deposited onto Au NPs can be controlled. The presence of acetonitrile in water helps to produce Au NPs with thin GC shells, which prevent nanoparticles growth and adhesion keeping some distance between neighboring nanoparticles. However, Au NPs prepared in water prone to aggregation, and there are no gaps between nearby nanoparticles. In this work, 10-3M 4-aminobenzenethiol (4-ABT) and 10-4M 4-nitrobenzenethiol (4-NBT) were chosen as Raman reports. The gap between nanoparticles – hot spot – is crucial for the SERS applications. The interparticle distance is found to be dependent on GC shell thickness controlled by solvent ratio. Therefore, SERS spectra intensity of analytes deposited on Au NPs prepared in mixture of acetonitrile and water is higher compare to that on Au NPs synthesized in pure water. Among all other samples, Au NPs ablated in 30 vol% of acetonitrile in water showed strongest SERS. Au NPs in this sample have appropriate size and sufficient amount of hot spots between nanoparticles to generate strong electromagnetic field. It allows this sample to meet the requirements of the ideal substrate. These Au NPs produced via facile way will allow promising prospects for detecting and analyzing biomolecules.

Poster Presentation : **PHYS.P-231**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Development of fluorescent 'Trun-On' type Pyrene-Schiff base based Mercury ion sensor derivatives

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We developed a new fluorescent turn-on type sensor based on pyrene-schiff base. Among various metal cations, the probe reacted selectively to mercury, and when irradiated through a fluorescence spectrophotometer, fluorescence increased when mercury ions and probes were combined. In addition, the probe operates smoothly at neutral and basic pH, and the detection change can be confirmed with the eye. Through the Job's plot experiment, it was found that the probe and mercury ions were bound by 2:1.

Poster Presentation : **PHYS.P-232**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Study on Ionic conductivity of silver-modified NASICON-type Li1.3Al0.3Ti1.7(PO4)3 solid electrolyte for all-solid-state lithium batteries

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NASICON-type Li1.3Al0.3Ti1.7(PO4)3 (LATP) oxide solid electrolyte shows high ionic conductivity and Li+ transfer number, favorable mechanical property, and excellent electrochemical and thermal stability. Silver was substituted to the Li1.3Al0.3Ti1.7(PO4)3 solid electrolyte by using a modified solid-state method for all-solid-state lithium batteries (ASSLB). The synthesis process of the material was divided by 3 chemical formulas from the different stoichiometric calculations. The pristine Li1.3Al0.3Ti1.7(PO4)3 was also synthesized for comparison before and after silver modification. X-ray diffraction patterns showed a similar peak with slightly increased and peak broadening for silver-modified LATP. There are also small new peak appeared at around 46-47 theta degree indicating that the modification of silver on LATP has successfully synthesized. Scanning electron microscopy of those samples confirmed the morphology of the solid electrolyte and shows the proportional silver ratio distribution. The ionic conductivity measurement was conducted by Electrochemical Impedance Spectroscopy (EIS). Pristine LATP without substitution shows the ionic conductivity around 0.1 mS/cm and the temperature dependence also measured to investigate the EIS properties at different temperatures. After that, the different silver-substitute LATP with different chemical formulas will further observe and optimized so it can be used for electrolyte for all-solid-state lithium-ion batteries.

Poster Presentation : **PHYS.P-233**
Physical Chemistry
Zoom 4 WED 17:30~18:00

Time-resolved spectroscopic study of a dynamically prototropic hydration probe in a reverse micelle

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The study of hydration dynamics in a reverse micelle (RM) have been studied to understand the phenomena in various confined systems.[1-3] We investigated the hydration dynamics in the nano-sized water pool of an Aerosol-OT (AOT) RM using a prototropic fluorescent dye, N-methyl-7-hydroxyquinolinium ($NM7HQ^+$), as the probe.[4] The size of water pool within the RM is controlled by size parameter w_0, where w_0 = [H_2O]/[AOT]. We intensively studied how the dynamic properties of the nano-sized water pool is affected at its interface with the anionic AOT headgroups by controlling $w_0$value.$NM7HQ^+$ is a photoacid exhibiting the decrease of its pKa value following photoexcitation. This results in the subsequent deprotonation of its excited-state cationic form (C*) giving rise to a keto species (K*) as the product. In the present study, the residence sites of C* and K* in the water pool were verified by monitoring time-resolved fluorescence anisotropy decay with the w_0 variation. Both the C* and K* bands evolving in time-resolved fluorescence spectra were analyzed by fitting the spectra to the sum of two log-normal peak functions. We focused on the time-dependent Stokes shift of each fluorescence band, as separated from that brought about by the excited-state proton transfer. The time-dependent spectral shift of each species of different formal charge revealed how the characteristic hydration behavior in the vicinity of the prototropic probe and their convection within the RM.Reference[1] *Biophys. J.* 2002, 82, 1570-1579.[2] *Enzyme Microb.* Technol. 1986, 8, 266-273.[3] *Eur. J. Pharm.* Biopharm. 2011, 79, 197-204.[4] *J. Mol. Liq.* 2020, in press.

Poster Presentation : **PHYS.P-234**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Photocarrier relaxation pathways and multi-exciton relaxation of CdSe nanorods

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With the advances in the topology study of the semiconductor nanocrystal, various designs of semiconductor nano-heterostructures, from organic molecules to metal hybrid structures and from 0D (nanodot) to 2D structures (nanosheet), have been extensively investigated for the future photovoltaics, biosensing, and energy harvesting materials.[1,2] For high catalytic and light-harvesting performance, the carrier dynamics of semiconductor nanostructures needs to be fully understood.Here, we systematically studied the photocarrier pathway of CdSe nanorods with the time-resolved absorption and emission spectroscopy spanning a wide time window (100's of fs to sub-μs). With the control of fluence and the wavelength of the excitation and the length of the nanorods, the combined time-resolved spectroscopic study deciphered that ultrafast intra-band relaxation (

Poster Presentation : **PHYS.P-235**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Filming Morphological Dynamics of Black Phosphorus Revealed in Ultrafast Electron Microscopy

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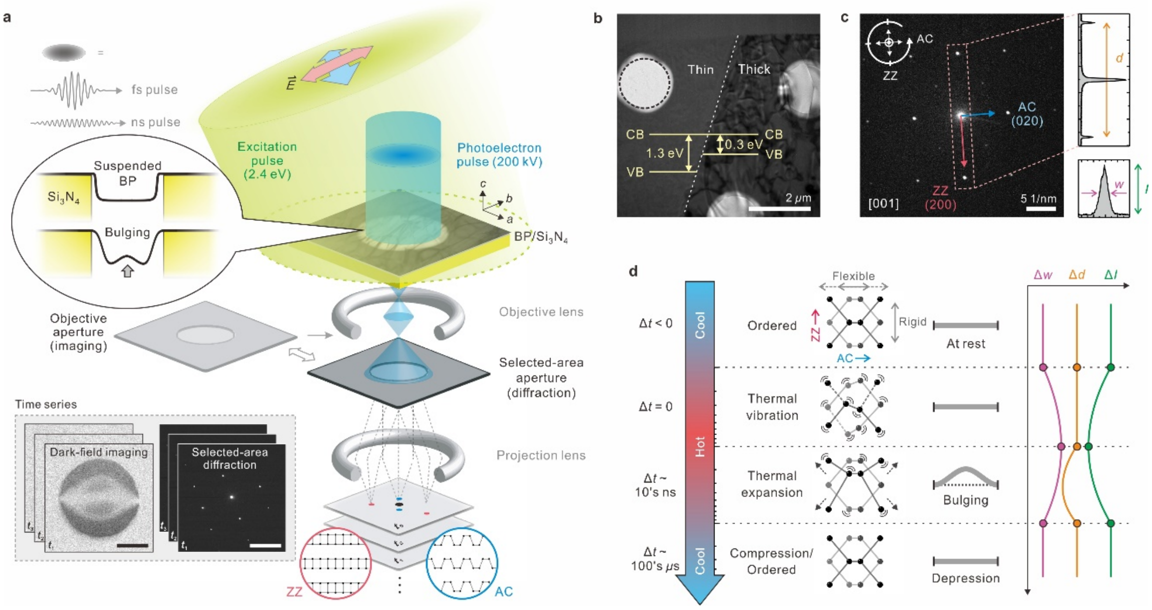
With the rapid development of two-dimensional (2D) matter, orthorhombic black phosphorus (BP), composed of puckered phosphorus layers via van der Waals interactions, recently has been widely studied due to its striking anisotropic properties [1]. Despite huge interests in BP from both fundamental and technical aspects [2], investigation into its structural dynamics induced by transient strain fields, prevalent for 2D materials and tuning the material physical properties, has been overlooked. Here, we track the course of the morphological deformation and relaxation of suspended BP membranes on timescales spanning nanoseconds to microseconds observed by time-resolved diffractograms and dark-field images in ultrafast electron microscopy (UEM) using pulsed photoexcitation as the source of brief thermal stress [3,4] (Figure 1). The number of BP layers, as well as the excitation polarization, fluence, and probe axis, were all controlled to analyze the anisotropic behavior. Aided by 4D structural reconstruction, we visualize the nonequilibrium bulging of thin BP membranes and reveal the buckling transition driven by impulsive thermal stress upon photoexcitation in real time. Finite element modeling was performed to simulate the stress and strain energy accompanied by the structural transition. The transient bulging, buckling, and flattening of the suspended BP membrane showed anisotropic spatiotemporal behavior. Because the strain field in the form of ripples and buckles on the surface of 2D matter modulates many physical properties, especially the optical and electrical properties, tailoring the transient anisotropic morphology of BP may allow fast spatiotemporal responses to light and unique multi-order functionality.[1] Ling, X., et al., Proc. Natl. Acad. Sci. U.S.A 2015, 112, 4523-4530.[2] Wang, Z., et al., Nano Lett. 2016, 16, 5394-5400.[3] Kim, Y.-J., et al., Matter 2019, 1, 481-495.[4] Kim, Y.-J., et al., ACS Nano 2020, https://doi.org/10.1021/acsnano.0c03644.


a
fs pulse
ns pulse
Suspended BP
Si3N4
Bulging
Excitation pulse (2.4 eV)
Photoelectron pulse (200 kV)
c
b
a
BP/Si3N4
Objective aperture (imaging)
Objective lens
Selected-area aperture (diffraction)
Projection lens
Time series
Dark-field imaging
Selected-area diffraction
t1
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ZZ
AC
b
Thin
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0.3 eV
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Δt < 0
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Δt ~ 10's ns
Δt ~ 100's μs
Cool
Hot
Cool
Ordered
Thermal vibration
Thermal expansion
Compression/ Ordered
Flexible
Rigid
ZZ
AC
At rest
Bulging
Depression
Δw
Δd
Δl

Poster Presentation : **PHYS.P-236**

Physical Chemistry

Zoom 4 WED 17:30~18:00

In Situ Generated Silver Nanodot Förster Resonance Energy Transfer Pair Reveals Nanocage Sizes

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Characterizing nanocages in macromolecules is one of the keys to understanding various biological activities and further utilizing nanocages for novel materials synthesis. However, fast and straightforward detection of the nanocage size remains challenging. Here, we present a new approach to detect the diameter of a nanocage by Förster resonance energy transfer (FRET) of luminescent silver nanodot pairs with reverse micelles as a model. Silver nanodot FRET pairs can be generated in situ from a single silver nanodot species with critical energy transfer distances, R0, of 4.8−6.5 nm. We have applied this approach to clarify the size variation of the water nanocage in nonionic surfactant Triton X-100- based reverse micelles. FRET efficiency decreases as more water is added, indicating that the size of the reverse micelles continuously expands with water content. The silver element in the nanocage also enhances the visualization of the nanocage under cryo-TEM imaging. The diameter of the water nanocage measured with the above approach is consistent with that obtained by cryo-TEM, demonstrating that the FRET measurement of silver nanodots can be a fast and accurate tool to detect nanocage dimensions. The above demonstration allows us to apply our strategy to other protein-based nanocages.

Poster Presentation : **PHYS.P-237**
Physical Chemistry
Zoom 4 WED 17:30~18:00

Ultrafast dynamics study of organosulfur molecule using x-ray absorption spectroscopy at PAL-XFEL

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Time-resolved X-ray Absorption Spectroscopy (TR-XAS) is powerful tool to probe time-evolving electronic and molecular structural dynamics in ultra-short timescale. For example, in S K-edge, it is sensitive to both the charge and the character of the low-lying valence orbitals in S atom. In this work, we investigated the early stage dynamics in proton transfer reaction of 2-Thiopyridone (2TP) in femtosecond time domain. 2TP complex is widely used in general chemical synthesis, antimicrobial and antifungal uses [1,2]. 2TP has a tautomer form, 2-mercaptopyridine (2MP) by proton transfer between S and C. Photoexcitation of 2TP which leads to the formation of 2MP was studied with 70-ps temporal resolution in our group using synchrotron, Advanced light source (ALS) [3]. We searched the early stage dynamics of photoreaction of 2TP by S K-edge TR-XAS at PAL-XFEL. PAL-XFEL is unique facility for tender X-ray (2~5 keV) TR-XAS in intensity. 2TP was excited by 400-nm fs laser pulse and 2.48 keV (S K-edge) XFEL was used as probe. Proton transfer reaction of 2TP was tracked with 150 fs temporal resolution.Our measurement shows the key spectral changes from 2TP to 2MP in several hundreds of ps time range which we've already found our previous measurement [3], and we picked up another short-lived intermediate at sub-ps time range. We estimate the short-lived intermediate as highly excited 2TP and the highly excited 2TP was relaxed to triplet state of 2TP within 1 ps. To support experiment result, we also calculate theoretical XAS spectra using time-dependent density functional theory. References[1] J. Am. Chem. Soc. 72, 4362–4364 (1950).[2] Selective Toxicity: The Physico-Chemical Basis of Therapy, 7th ed. (Chapman and Hall, London, 1985).[3] Struct. Dyn. 4, 044021 (2017)

Poster Presentation : **PHYS.P-238**
Physical Chemistry
Zoom 4 WED 17:30~18:00

Substructure-based Neural Machine Translation for Retrosynthetic Prediction

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With the rapid improvement of machine translation approaches, neural machine translation has started to play an important role in retrosynthesis planning, which finds reasonable synthetic pathways for a target molecule. Previous studies showed that utilizing the sequence-to-sequence frameworks of neural machine translation is a promising approach to tackle the retrosynthetic planning problem. In this work, we recast the retrosynthetic planning problem as a language translation problem using a template-free sequence-to-sequence model.The model is trained in an end-to-end and a fully data-driven fashion. Unlike previous models translating the SMILES strings of reactants and products, we introduced a new way of representing a chemical reaction based on molecular fragments. It is demonstrated that the new approach yields better prediction results than current state-of-the-art computational methods.The new approach resolves the major drawbacks of existing retrosynthetic methods such as generating invalid SMILES strings. Specifically, our approach predicts highly similar reactant molecules with an accuracy of 57.7%. In addition, our method yields more robust predictions than existing methods.

Poster Presentation : **PHYS.P-239**

Physical Chemistry

Zoom 4 WED 17:30~18:00

Scattering of adiabatically aligned molecules by nonresonant optical standing waves

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We study the effect of rotational state-dependent alignment in the scattering of molecules by optical fields. CS_2 molecules in their lowest few rotational states are adiabatically aligned and transversely accelerated by a nonresonant optical standing wave. The width of the measured transverse velocity distribution increases to 160 m/s with the field intensity, while its central peak position moves 10 to -10 m/s. These changes are well reproduced by numerical simulations based on the rotational state-dependent alignment but cannot be modeled when ignoring these effects. Moreover, the molecular scattering by an off-resonant optical field amounts to manipulating the translational motion of molecules in a rotational state-specific way. Conversely, our results demonstrate that scattering from a nonresonant optical standing wave is a viable method for rotational state selection of nonpolar molecules.

Poster Presentation : **ANAL.P-240**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Detection of Symmetric Dimethylarginine by competitive single-site immunometric assay and avidin/biotin system

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Symemetric Dimethylarginine (SDMA) is the structural isomer of the endogenous nitric oxide synthase inhibitor, asymmetric dimethylarginine (ADMA). Creatinine was the most common bio-marker of renal function, specially the glomerular filtration rate (GFR). But, several studies show that the concentration of SDMA increases before the creatinine does when there is renal dysfunction. And creatinine shows instability being affected by non-renal function factors. Thus, sensitive detection of SDMA can be used as a new bio-marker of chronic kidney disease (CKD). Single-site immunometric assay is an immunological technique with several advantages as sensitivity, simplicity, and specificity. This method is used when target's epitope is estimated to be one. To detect SDMA quantitatively, free SDMA was coupled to bovine serum albumin (BSA). It is synthesized by activating the carboxyl group of BSA and the amino group of the SDMA using EDC method. The initial ratio of SDMA-BSA conjugate is 1:100 (BSA:SDMA). The synthetic material acts as a competitor to the target. After a competitive reaction, quantitative analysis is possible using avidin/biotin system. Anti-SDMA antibody conjugated biotin and avidin conjugated horseradish peroxidase (HRP) are involved. HRP produces a detection signal and enables quantitative analysis of the target material.Thus, we expect that this study will advance the detection of SDMA as a novel marker of renal function.

Poster Presentation : **ANAL.P-241**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Amplification-free detection of COVID-19 target genes using a SERS-based microdroplet chip

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The coronavirus disease 2019 (COVID-19) outbreak has been labelled an ongoing pandemic by the World Health Organization (WHO). Real time quantitative polymerase chain reaction (RT-qPCR) has been recently considered a gold standard for the quantitative evaluation of a target gene but it still suffers from the problem of a long thermocycling time. To address this issue, we developed a surface-enhanced Raman scattering (SERS)-based DNA detection platform for the rapid and sensitive detection of target DNA markers of corona virus. Just like the RT-qPCR, two DNA probes, a broad-range probe for E gene and an additional probe for RdRp gene, have been used for the simultanelous detection two target DNAs of corona virus. The Raman signals of DNA markers were measured under flowing conditions. Total analysis time from droplet generation to SERS detection takes less than 10 min because all experimental conditions are automatically controlled inside the exquisitely designed microfluidic channel. This novel SERS-based DNA sensing technology in a microdroplet channel is expected to be a powerful analytical tool to simultaneously detect multiple DNA oligomer markers of infectious disease.

Poster Presentation : **ANAL.P-242**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

Effective determination of chiral nicotine using Dispersive Liquid-Liquid Microextraction HPLC/UV-vis

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Nicotine is a stimulant and powerful alkaloid, usually derived from tobacco plants, but this nicotine can also be obtained through chemical synthesis. In the case of natural nicotine, the content of (S)-nicotine is overwhelmingly higher than that of (R)-nicotine. Synthetic nicotine is mainly used for e-liquid production. In this study, we performed an improvement of the nicotine extraction method using DLLEME to differentiate between natural nicotine and synthetic nicotine and to effectively separate chiral nicotine. In order to optimally extract nicotine from each sample, the sample using high performance liquid chromatography (HPLC) / UV-Vis after comparing the type of dispersion solvent, pH, and amount of salt that can be used in DLLME to obtain optimal efficiency. optimally Established a method to separate and quantify chiral nicotine.. Experiments were conducted to confirm the matrix effect and to determine the optimal solvent conditions. Chromatographic separation using HPLC/UV-Vis was performed using a CHIRALCEL OD-H (4.6 mm id x 250 mm length, 5 μm particle size) column and isocratic conditions with hexane and ethanol. By using this method, chiral nicotine present in the sample is extracted more efficiently, enabling quantitative and qualitative analysis.

Poster Presentation : **ANAL.P-243**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

Size sorting of extracellular vesicles from cell using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

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Extracellular vesicles (EVs) are cell-derived membrane-covered particles containing proteins, lipids, nucleic acids and other biological molecules. EVs play an essential role in the communication between cells via transporting pathologically important molecules. As the pathological importance of EVs increases, the expectation of EVs as a biomarker is growing. Subpopulations of EVs are divided into exosomes (30-100 nm in diameter) and microvesicles (100-1000 nm) according to their sizes and therefore, it is important to separate them because they differ in cellular origins, contents, and lipid compositions. However, it is challenging to isolate EVs while each of the separation methods such as ultracentrifugation, size exclusion chromatography, filtration, and precipitation has its own limitation.Field-flow fractionation (FFF) is a separation method capable of fractionating particles from nano to micron size in aqueous solution without using packing materials. In this study, exosomes and microvesicles secreted from cells were separated by frit-inlet asymmetrical flow field-flow fractionation (FI-AF4) with field programming and monitored by UV and multi-angle light scattering (MALS) detectors. Eluted exosomes and microvesicles were identified by western blotting and their sizes were determined by MALS and dynamic light scattering (DLS). Further, 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.

Poster Presentation : **ANAL.P-244**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Flow field-flow fractionation with thickness tapered channel

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Flow field-flow fractionation (FlFFF) is a separation method that is capable of fractionating particulate or macromolecules by the differences in the hydrodynamic diameters of sample components in an empty channel space. FlFFF utilizes two perpendicular flow streams: migration flow to drive sample components to migrate along the channel and crossflow to retain sample materials within the channel. In general, separation is achieved by the increasing order of diameter typically in the normal operating mode and it useful to separate biological macromolecules or particles with broad molecular weight or diameter distribution. While separation efficiency in FlFFF increases with the increase of channel thickness, it increases the separation time and often induces poor recovery of long retaining components such as large MW or diameter species. To overcome this issue, FFF has been commonly utilized with field programming method in which the field strength gradually decreases with time so that retention time can be shortened with the increase of sample recovery and resolution. However, additional hardware to control the two flow rates is required for the programming of the field strength in FlFFF. In this study, a new type of channel with tapered thickness for asymmetrical flow field-flow fractionation is introduced. Thickness tapered channel exhibits a field programming effect without any software or instrument owing to the increasing migration flow velocity along the channel axis. Separation efficiency of the thickness tapered channel was investigated in various flow rate conditions by comparing retention time, peak width, and peak height to those of the channel with uniform thickness.

Poster Presentation : **ANAL.P-245**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Microfluidic analytical device for Nucleic Acids Amplification and Detection

Nguyet mai Ly, Veasna Soum, Nayoon Pyun, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Polymerase chain reaction (PCR) for nucleic acid amplification plays an important role in genetics study as well as practical applications in diagnosis and detection, quality control, and quantitative monitoring of diseases, pathogens, or potential biomarkers. Conventional PCR is limited by time, equipment, tools, and skills of technicians. Many research groups have aimed to miniaturize PCR into a lab-on-chip device for point-of-care testing (POCT). Traditional approach is to use heating blocks with microfluidic device on which the flow is controlled by a supportive pumping system. To avoid dependence on pump, here we plan to build up a pumpless PCR chip controlled by capillary flow for self-regulated liquid delivery. Additionally, the flexible printed heaters on polyimide film fabricated by inkjet printer using conductive nano-silver ink have been provided for the underneath heating bed. For simple detection and easy visualization of amplified PCR products, a lateral flow assay will be employed later. This comprehensive device will promise a portable platform for POCT, being capable to complete both amplification and detection of target nucleic acid.

Poster Presentation : **ANAL.P-246**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

Effect of reduced Graphene oxide and $MnFe_2O_4$ nanoparticles on Carbonyl Iron for Magnetorheological Fluids

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Magnetorheological(MR) fluids are colloidal suspensions of magnetic particles dispersed in non-magnetic liquid medium such as silicone oil. They change from a fluid-like to a solid-like structure under an external magnetic field, resulting in a significant increase in shear viscosity, yield stress, and dynamic modulus. Carbonyl iron(CI) particles have been used as magnetic materials for MR fluids due to their proper particle size and high saturation magnetization, but they cause serious sedimentation problems in MR fluids. To solve this problem, two different kinds of additives were introduced to the CI solution in this study. Graphene oxide(GO) is expected to improve the dispersion and sedimentation stability of MR fluids due to its low density, planar structure and large specific surface area. $MnFe_2O_4$ is also expected to improve distributed stability and magnetorheological characteristics because it has high magnetization rate, low density and distinct magnetism. The aqueous CI solution was first mixed and sonicated with sodium hydroxide and GO, and then transition metal solutions of manganese(II) nitrate and iron(III) chloride was slowly added to the CI solution, preparing in CI/ $MnFe_2O_4$/GO. The final product, CI/ $MnFe_2O_4$/rGO, was synthesized by annealing to reduce GO to rGO. The CI/$MnFe_2O_4$/rGO was dispersed to the silicon oil by ultrasonication. The morphologies, compositions and crystal qualities of the prepared CI/$MnFe_2O_4$/rGO composites were characterized by SEM, EDS, TEM, XRD and XPS. The magnetic properties of CI/$MnFe_2O_4$/rGO were measured using a VMS. The MR performances of the prepared MR fluids were investigated by a rotating rheometer.

Poster Presentation : **ANAL.P-247**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

Synthesis and application of CNFs/GQD/SiNPs and CNT/GQD/SiNPs composites as anodes for Lithium-ion batteries

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[1]*Department of Applied Chemistry, Andong National University, Korea*

We used graphene quantum dots instead of graphite, which is one of the most popular anode material for existing lithium ion batteries. Silicon nanoparticles (SiNPs) and carbon nanomaterials are introduced to synthesize carbon nanofibers/graphene quantum dots/silicon nanoparticles (CNFs/GQD/SiNPs) and carbon nanotubes/graphene quantum dots/silicon nanoparticles (CNT/GQD/SiNPs) composites to improve their low capacity of carbon materials. To fabricate these composites, we positively charged SiNPs by adding poly(diallyldimethylammonium chloride)(PDDA). Subsequently, we combined the positively charged SiNPs with OH-GQDs using electrostatic attraction followed by mixing and dispersing the GQD/SiNPs nanocomposites with CNFs and CNT, respectively. After stirring, we filtered and dried the composites in the oven. The composites are reduced through annealing under Ar/H2 gases. The finally produced material is assembled into a coin cell to test battery performance which undergoes CV, rate capability, cycling test, and EIS. Before blending carbon nanomaterials, the discharge capacity of GQD/SiNPs composites is approximately 811.8mAh/g after 100 cycles. In addition, the prepared materials are characterized to investigate their physical properties via SEM/EDS, TEM, XRD, XPS, Raman, and FT-IR. We expect that these composites not only increase charging capacity, but also enhance the overall performance of the batteries by complementing each components' shortcomings.

Poster Presentation : **ANAL.P-248**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

SERS-based immunoassay of thyroid-stimulating hormone (TSH) using silver-encapsulated gold nanoparticles and fabrication of 3D paper fluidic chips

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Thyroid-stimulating hormone (TSH) is essential for regulating the body`s metabolism and is also used as a biomarker for the diagnosis of hyperthyroidism (inhibited) and hypothyroidism (elevated). Lateral flow assay (LFA) strips can be used for the diagnosis of hypothyroidism but there is no commercially available one for hyperthyroidism since it is difficult to detect an extremely low TSH concentration in human serum. Radioimmunoassay (RIA), immunochemiluminescent assay (ICMA) and enzyme-linked immunosorbent assay (ELISA) methods are used to detect TSH below the normal range from 0.5 to 5 uIU/mL but they have several drawbacks including a long assay time and high cost. Herein, we report the fabrication of a conceptually new 3D paper fluidic chip and the production of silver-encapsulated Au nanoparticles (Ag-AuNPs) for highly sensitive detection of TSH. Ag-AuNPs generate hot spots at the nanogaps between Ag shell and Au core, and consequently induce a greatly enhanced Raman signals. It is possible to diagnose hyperthyroidism as well as hypothyroidism since a TSH concentration lower than 0.5 uIU/mL can be detected using these techniques. We believe that this approach can be also used for the diagnosis of other hormones that require high sensitivity.

Poster Presentation : **ANAL.P-249**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

Synthesis of Red Luminescence Carbon dot by Eu^{3+} and Detect Method

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Carbon quantum dot (CQD) is a new class of Carbon based fluorescent nano materials (less than 10nm in size), which has recently attracted considerable attention due to their superior properties of stability, bio-compatibility, low toxicity, good water solubility. The luminescent properties of CQD depend on the funtional groups contained on their surfaces. The lanthanide based luminescent nano structures have been recognized for their better chemical and optical properties originating from their electronic structures of *f*-orbital electrons. Europium has red luminescent fluorescence and sharp peak characteristic at 615nm($^5D_0 \rightarrow {}^7F_2$) of line type red *f-f* emission. Research for Eu^{3+}-modified CQD has been actively pursued because it is soluble in water and has a wide range of applications : light-emitting diode, organic lgith-emitting diode, bioimaging, sensing and targeting specific DNA structures.In during of CQD synthesis, we tried to combine Eu but the Eu^{3+} emission is rapidly quenched by water for OH^-. Several papers have found that using β-diketone caused complexing with Eu and could prevent Eu from losing a red light. When composing CQD, Eu was added, β-diketone was used to block OH^- ions, and the red light from Eu-CQD under UV lamps was finally determined. Also the width peak under UV lamps was measured at a rapid peak of λ_{em}=615nm in the expiratory spectrum. By introducing this method, the carbon dots that combine Europium are expected to be used in various filed today.

Poster Presentation : **ANAL.P-250**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Electrochemical sensing of dopamine using nanoparticle composites modified screen-printed carbon electrode in human urine sample

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Dopamine is an essential neurotransmitter that plays an essential role in our physical body including emotion, appetite, thought, and so on. Therefore, it is of great necessity to develop a new method for sensing of dopamine in human biological samples. In this poster, we demonstrated a sensitive and selective electrochemical sensor for DA analysis using poly(L-methionine), carbon nanotube-graphene complex, and electrodeposited Au nanoparticles on screen printed carbon electrode surface. The surface morphology of our sensor was investigated by FE-SEM, EDS, and XPS while the electrochemical performance was examined by cyclic voltammetry and differential pulse voltammetry. The developed sensor was also applied to the human urine sample and compared with that of LC-MS results.Keywords: electrochemical sensor, carbon nanotube-graphene, dopamine.

Poster Presentation : **ANAL.P-251**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Electrochemical Layer-by-layer biosensors for hypoxanthine and inosine in human serum sample solutions

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In this poster, we demonstrated two layer-by-layer (LbL) electrochemical biosensors for myocardial ischemia biomarkers hypoxanthine (HX) and inosine (INO) in both buffer and human serum samples. For HX, poly(diallyldimethylammonium chloride) wrapped carbon nanotube-graphene complexes and negatively charged xanthine oxidase assembled on screen printed carbon electrode was developed [1] while chitosan and purine nucleoside phosphorylase were for INO sensor fabrication [2]. Our LbL sensing platforms were applied to the concentration analyses of HX and INO in human normal and myocardial infarction patient serum samples. The electrochemical sensing results of HX were compared to those obtained from liquid chromatography-mass spectrometry (LC-MS) while INO results to LC-MS and an assay kit.Keywords: layer-by-layer, electrochemical biosensor, hypoxanthine, inosine, serum References[1] Y. Si, J.W. Park, S. Jung, G.S. Hwang, E. Goh, H.J. Lee, Layer-by-layer electrochemical biosensors configuring xanthine oxidase and carbon nanotubes/graphene complexes for hypoxanthine and uric acid in human serum solutions, Biosens Bioelectron, 121(2018) 265-71.[2] Y. Si, J.W. Park, S. Jung, G.-S. Hwang, Y.E. Park, J.E. Lee, H.J. Lee, Voltammetric layer-by-layer biosensor featuring purine nucleoside phosphorylase and chitosan for inosine in human serum solutions, Sens Actuators B Chem, 298(2019) 126840.

Poster Presentation : **ANAL.P-252**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

SERS-PCR assays of SARS-CoV-2 using three-dimensional plasmonic nanodimple substrates.

Yixuan Wu, Jaebum Choo*

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As evident from the ongoing COVID-19 pandemic, a rapid and accurate diagnosis of infectious diseases is crucial for effective prevention of disease spread. Real-time polymerase chain reaction (RT-PCR) technique is considered as a current gold standard for diagnosis of SARS-CoV-2. Fluorescence detection method using TaqMan probes is used for the detection of terget genes after 30-40 thermocycling steps in RT-PCR. However, it often lacks the detection sensitivity for rapid and accurate detection of terget genes. Therefore, it is important to develop a sensitive detection method to reduce the time for diagnosis of SARS-CoV-2. Herein, we report a surface-enhanced Raman scattering based polymerase chain reaction (SERS-PCR) assay platform for the rapid detection of SARS-CoV-2. To enhance the Raman signals, three-dimensional nano-dimple plasmonic substrates were employed as a SERS assay platform. It was possible to detect the target gene at 32 copies/μL level after 20 PCR cycles by the SERS-PCR, while it takes approximately 40 PCR cycles to detect a target gene by RT-PCR. Thus, this SERS-PCR demonstrates a strong potential to be used as a rapid detection method for diagnosis of SARS-CoV-2.

Poster Presentation : **ANAL.P-253**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Method Validation of N-nitrosodimethylamine in Diltiazem by UPLC-ESI-SRM/MS

Keewon Yang, Jae-ung Lee[1], Han Bin Oh[1,*]

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In 2018, N-nitrosodimethylamine (NDMA) was first found in Valsartan, which is a drug used for treating hypertension. Since then, NDMA has been discovered in other drugs like Ranitidine and Metaformine. International Agency for Research on Cancer (IARC) classified NDMA as '2A' type chemical, which is a chemical that may act as a carcinogen over ingestion. Different approaches, like GC-MS/MS, thermal desorption GC-MS and LC-MS/MS, were used to identify and quantify NDMA in different drugs and products. In this study, a method validation on NDMA in Diltiazem using the UPLC-ESI-SRM/MS was carried out to see if the method satisfies the guideline suggested by the KP/ICH and Ministry of Food and Drug Safety. Different criteria, like system suitability, specificity, linearity, accuracy, precision, limit of detection (LOD), limit of quantitation (LOQ) and robustness, were verified. Specificity of NDMA was tested for standard solutions prepared in methanol and two different matrices, capsule and tablets, which turned out to be no difference between the matrices. LOD and LOQ for NDMA in standard solution were 0.1 ng/mL and 2 ng/mL, respectively. The correlation coefficient (R2) of the linear regression line obtained in the concentration range of 2–100 ng/mL was 0.9992. The accuracy and precision of the method were also satisfied. In the future study, inter-laboratory precision and robustness of the method will be verified for drug substances and drug products.This research was supported by Ministry of Food and Drug Safety (20173MFDS162).

Poster Presentation : **ANAL.P-254**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Identification of cervicovaginal fluid metabolites associated with preterm birth

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Western Seoul Center, Korea Basic Science Institute, Korea

Preterm birth (PTB) is defined as fetal birth less than 37 weeks of pregnancy, and is a serious problem of the neonate and maternal health with the risk of mortality and morbidity. During pregnancy, there are physiological changes, such as the interaction between the maternal microbiota and the fetus environment, which affect the composition of the vaginal microbial cluster. To date, very limited studies are available that have examined the putative microbiota metabolites for preterm birth. Thus, it is necessary to find specific biomarkers that can predict preterm birth for an in-depth understanding of the vaginal microbiota metabolites inducing preterm birth. In this study, we analysed vaginal microbiota metabolites to identify markers that can predict preterm birth compared to term birth. We performed metabolic profiling using nuclear magnetic resonance (NMR) spectroscopy to investigate metabolites in cervicovaginal fluid (CVF) samples from pregnant women with preterm birth and term birth. The 8 metabolites were significantly increased in the preterm birth group compared with the term birth group, and these metabolites could be beneficial markers for clinical application of preterm birth predictions.This study demonstrates certain CVF metabolites have shown significant changes in the preterm birth compared to term birth and metabolomics approach can be used to investigate markers predicting preterm births.

Poster Presentation : **ANAL.P-255**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Surface Activated NiFeOx Nanosheets for Enhanced OER Catalysis

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[1]*Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Korea*

Currently, the electrolysis of water to form hydrogen as an option to store surplus renewable energy sources such as solar and wind has drawn the attention of many research institutions and industries. However, the efficiency of water electrolysis is hampered by the slow kinetics of the anodic OER in alkaline electrolytes. Ni-Fe based materials have been acknowledged for OER catalysts because of their earth abundance, better activity, and stability in strong electrolytes. However, they still suffer from low conductivity limiting their OER catalytic activity. Herein, we have investigated the OER activity of a series of Fe-doped Ni-based (oxy)hydroxide nanosheets synthesized by electrodeposition on to Nickel foam. Upon cycling in Fe-spiked electrolyte, Ni75Fe25/NF has exhibited higher OER current and low Tafel slopes in the range of 41 mV/dec in 1M KOH. However, in Fe-free electrolyte, Ni75Fe25/NF demonstrated low current density and higher Tafel slopes in the range of 65 mV/dec. Therefore, the inclusion of Fe post-deposition have significantly contributed to enhancing the OER activities of Ni100-xFex nanosheets.

Poster Presentation : **ANAL.P-256**

Analytical Chemistry

Zoom 5 WED 16:30~17:00

Serum metabolic profiling in morbid obese patients after bariatric surgery using NMR and LC/MS

Yeyoung Han, Do Hyun Ryu[1,*], Geum-Sook Hwang[*]

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Bariatric surgery is one of the most effective treatments for obesity and its complications. However, metabolic changes in bariatric surgery are not clear. In this study, we performed metabolic profiling of serum from 38 morbid obese patients who underwent bariatric surgery using nuclear magnetic resonance spectroscopy (NMR) and liquid chromatography/ mass spectrometry (LC/MS). We integrated metabolic profiling and gut microbiota profiling data to observe changes in human metabolism and intestinal environment after bariatric surgery. Samples were collected before surgery and 6 months after surgery. In global profiling using NMR, metabolites including amino acids, organic acids, carbohydrates, and short chain fatty acids were identified in serum of patients. Principal component analysis (PCA) score plot showed a clear separation between before surgery and after surgery group. We found that serum metabolites associated with obesity metabolism (branched-chain amino acids (BCAAs) and aromatic amino acids) and metabolites related to energy metabolism (glucose, glutamate, lactate, and mannose) were significantly decreased after surgery. Interestingly, BCAAs, glucose, and mannose were positively correlated with total cholesterol, LDL cholesterol, triglyceride, which are clinical indicators related to lipid metabolism. In correlation analysis of metabolome and gut microbiome, BCAA metabolites were positively correlated with *Roseburia faecis*. Glycine and dimethyl sulfone were related to *Streptococcus infantis* and *Rothia dentocariosa*. In addition, we performed a quantitative analysis of serum bile acids (BAs) using LC/ triple quadrupole MS (LC/TQ-MS) to measure the level of circulating bile acids reabsorbed in the intestine. After surgery, the total level of BAs increased compared to before surgery. Particularly, GDCA, TDCA, LCA, GLCA, and TLCA, which are secondary BAs, significantly increased after surgery, while primary BAs had little change. This study demonstrates that NMR/MS-based metabolic profiling analysis and it's integration with microbiome data provides insight into the metabolic changes after bariatric surgery.

Poster Presentation : **ANAL.P-257**
Analytical Chemistry
Zoom 5 WED 16:30~17:00

Surface Modified Hematite Photoanodes with NiFeOOH for Enhanced Solar Water Splitting

<u>Sohyun Kang</u>, Birhanu Bayissa Gicha[1], Jaebeom Lee[*]

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

The integration of earth-abundant active oxygen evolution catalysts (OECs) with diverse photoanodes are very important to realize the efficient photoelectrochemical (PEC) water splitting. Hematite is a suitable candidate for photoelectrochemical water splitting due to its well-suited band structure, stability, and availability. However, rapid charge recombination and slow water oxidation kinetics are key drawbacks that limit the photoelectrochemical water splitting efficiency of Fe2O3. Herein, we modify the surface of Fe2O3 photoanode by a bimetallic oxyhydroxide NiFeOOH layer in order to build highly matched semiconductor/cocatalyst interface. Benefited from the accelerated OER kinetics and low overpotential of bimetallic oxyhydroxide NiFeOOH, the resultant Fe2O3/NiFeOOH heterojunction interface possesses better visible light absorption, enhanced photocurrent density (1.50 mA/cm2 at 1.23 VRHE) and good stability than bare Fe2O3 and semi-FeOOH or NiOOH decorated Fe2O3 photoanodes.

Poster Presentation : **ANAL.P-258**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

An Untargeted Analysis of Metabolite Biomarkers in Urine for Miscarriage/Pre-term Birth using LC-MS/MS

Sae Yoon Oh, Han Bin Oh*

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Miscarriage is a birth-related issue that carries a pregnancy loss before 20 gestational weeks of pregnant women. According to Ministry of Health and Welfare of Korea, the rate of preterm birth in Korea has increased double in 2017 compared to the rate in 2000. There have been different approaches to find possible biomarker candidates, like proteins and lipids, related to miscarriage in urine, serum and plasma of pregnant women. However, no biomarker candidates related to preterm birth or miscarriage were identified, and more comprehensive search for the possible biomarker is required for metabolites and metabolic by-products.In this study, a dansyl reaction was utilized to search for metabolic biomarkers, which derivatizes various metabolites in urinary sample from pregnant women and patients experienced miscarriage. In the dansyl reaction, metabolites and metabolic by-products with amines and phenol functional groups could be derivatized using dansyl chloride and those with carbonyls and carboxyl functional groups could be labeled with dansyl hydrazine. We plan to identify and quantify derivatized metabolites in urinary samples using liquid chromatography tandem mass spectrometry (LC-MS/MS). Also, other metabolites like lysine, tyrosine and citrate were analyzed quantitatively as well. A deuterated internal standard for each metabolite was spiked into each urine sample and creatinine were also analyzed to precisely quantitate the metabolites in each urine samples. This research was supported by the Ministry of Health and Welfare of Korea (HI17C1238).

Poster Presentation : **ANAL.P-259**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Combined Exposure Assessment of Quaternary Ammonium Compounds (QACs) in Various Consumer Chemical Products (CCPs)

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Various biocidal chemicals included in the consumer chemical products (CCPs) have sacrificed many lives and impacted greatly on human health. To effectively regulate the chemicals in the CCPs, the Ministry of Environment have begun to strengthen the regulations on the usage of biocides in the CCPs. One of the most widely used biocidal chemicals in CCPs are quaternary ammonium compounds (QACs). QACs are a group of chemicals having a structure of NR4+, positively charged nitrogen atom with four alkyl chains (R) covalently connected to it. In this research, an analytical method using liquid chromatography tandem mass spectrometry (LC-MS/MS) were applied to identify and quantify 2 different QACs, benzylalkyldimethylethylammonium chloride (BAC), alkyltrimethylammonium bromide (ATMAB). To carry out the exposure assessment, the guidelines suggested by the US Environmental Protection Agency (US EPA) and Korea Ministry of Environment were followed to specify the exposure routes and scenarios. In this research, two different exposure routes, ingestion and dermal contact, were investigated to estimate how much QACs a person is exposed to while using CCPs. QACs in 4 different CCPs, fabric softener, mouthwash, eyedrop and hand sanitizer, were identified and quantified using LC-MS/MS. Furthermore, exposed amount of QACs through various routes were investigated, so that the overall assessment of body exposure to the QACs in the CCP could be estimated.AcknowledgementThis research was supported by a grant (2018002490001) through the Technology Program for Establishing Biocide Safety Management, funded by the Korea Environmental Industry & Technology Institute.

Poster Presentation : **ANAL.P-260**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Development of a screening software for the identification of unknown narcotic drugs using artificial intelligent approach and hybrid similarity search

So Yeon Lee[*], **Han Bin Oh**[1,*]

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A software for screening unknown narcotic drugs using the artificial neural network calculations and hybrid similarity search (HSS) algorithm was developed. Furthermore, identification of unknown narcotic drugs was carried out by simply comparing the mass spectra obtained by LC-MS/MS with the tandem mass spectra in the pre-constructed inhouse database. As similar structural analogues that do not affect the characteristics of narcotic drugs have recently increased to avoid drug screening, the number of substances that do not exist in the database has increased, making the screening of illicit analogues extremely difficult. To solve this challenge, we developed a screening software using the HSS algorithm and an artificial neural network model for narcotic drugs. The screening process using HSS algorithm is carried out by shifting the peak in the database by Deltamass(△m) to match the precursor m/z value of an unknown substance in the acquired tandem mass spectra. Using this approach, unknown analogues could be identified even when the database does not cover the substance under investigation.This research was supported by a grant (12208118500) through the funding by the Supreme Prosecutors' Office of the Ministry of Justice.

Poster Presentation : **ANAL.P-261**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Synthesis and structural studies of $LiFe_{1-x}Mn_xBO_3$ and $LiFe_{1-x}Co_xBO_3$ as a cathode material for Li–ion battery

Inyoung Lee, Youngil Lee[1,*]

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Successful operation of secondary Li-ion battery (LIB) relies on high-performance cathode materials that control the cost and energy density. Thus, battery community has been focused on discovery and development of cathode materials. These days, the cathode materials can be divided into two categories: lithium metal oxide and polyanionic compounds. Polyanionic structure compounds are widely studied as a cathode material for LIB. Among them, lithium metal borate ($LiMBO_3$, M= Mn, Fe or Co) forms have the lowest weight, thus offering the highest theoretical capacity (220 $mAhg^{-1}$). Also, the energy density is expected to be higher than phosphates. Among borate based materials, $LiMnBO_3$ has high operating potential, while $LiFeBO_3$ has high theoretical capacity. And $LiCoBO_3$ has the excellent combination of high theoretical capacity (215 $mAhg^{-1}$) and expected 4 V operation. Therefore, $LiFe_{1-x}Mn_xBO_3$ and $LiFe_{1-x}Co_xBO_3$ (x = 0, 0.25, 0.5, 0.75, and 1.0) composite materials have been synthesized with solid-state reaction method for structural studies according to the amount of electrons on metal sites. The morphology and structural studies of synthesized materials have been identified X-ray diffraction (XRD) and ^7Li MAS NMR. Also, quantitative analysis for the ratio of Mn : Fe and Fe : Co has been performed with laser induced breakdown spectroscopy (LIBS).

Poster Presentation : **ANAL.P-262**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Structural and electrochemical studies of $LiFeBO_3$ as a cathode material for lithium-ion battery

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Lithium iron borate, $LiFeBO_3$, is a particularly desirable cathode material for lithium-ion batteries because of its appealing chemical components, which are inexpensive and non-toxic and its high theoretical capacity of 220 mAh g^{-1}. However, it has low electrical conductivity due to its structural characteristics. Fluorine substitution at the oxygen sites of $LiFeBO_3$ to increase its conductivity and improve electrochemical properties has been studied with phase transition from monoclinic to vonsenite, in previous study. But after the first charge/discharge cycle, it indicate a dramatic decrease of capacity. So, we are studying to improve the stability of its structure by coating at the surface of $LiFeBO_{3-x}F_{2x}$ with maintaining high discharge capacity. The surface coated $LiFeBO_{3-x}F_{2x}$ have been synthesized by solid-state method and characterized by X-ray diffractometry (XRD), TEM images and ^{7}Li MAS NMR spectroscopy. The electrochemical properties of surface coated $LiFeBO_{3-x}F_{2x}$ have been measured by using Galvano static charge/discharge test with the potential range of 1.0 - 4.5 V.

Poster Presentation : **ANAL.P-263**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Synthesis and Electrochemical Properties of Sulfate-based Yavapaiite-like Structure for Promising Polyanionic Cathode Material

Reyhan Puji Putranto, **Youngil Lee***

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Domination of lithium-ion batteries (LIBs) have become sophisticated for electrical energy storage technology. However, depending on their applications, development of new electrode materials for LIBs especially with polyanionic compound needs to fulfill aspects such as high gravimetric and volumetric energy density, low-cost, charge/discharge rate, safety issues, and term of sustainability. Despite of $LiFePO_4$ as well-known cathode material, $Li_2V_2(SO_4)_3$ and $Li_2VO(SO_4)_2$ are shown good evidence of inductive effect for polyanionic material such as borate, phosphate, and silicate. In this study, novel lithium vanadium sulfate-based polyanionic cathode material via low temperature eco-efficient solution method has been developed. Electrochemical reversibility of active material has been conducted by 2016-coin cell with range of operating voltage 3.0 V – 4.8 V. X-ray diffraction pattern and infrared spectra support structural characterization of the material. Electrochemical performance of the first discharge has been obtained 36.45 mAh/g with C/20 rate. High potential of 3.85 V to extract Li-ion and charge voltage of 4.3 V for re-insertion process have been used.

Poster Presentation : **ANAL.P-264**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Sensitive and Selective Detection of Trace Metal Ion with Molecular-Like Au Clusters

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Gold nanoclusters (Au NCs) are a class of ultra-small size of nanoparticles, which usually consists of several to tens of atoms, have been developed and stimulated extensive interests due to the molecular like properties such as fluorescence, high surface area, and stability. So far, Au NCs have been widely used as fluorescent probes for the detection of various metal ions with trace concentration. The interaction between metal ions and Au NCs, which capped with a negatively charged molecules, leads different fluorescent properties of Au NCs depending on the types of metal ions, and the fluorescence property of Au NCs might also be manipulated by the kinds of the capping agent. In this research, we investigated the interaction between the Glutathione capped-Au NCs and various metal ions such as Al^{3+}, Zn^{2+}, Cd^{2+}, Pb^{2+}, Ag^{+}, Ca^{2+}, Mn^{2+}, Ni^{2+}, Cr^{3+}, Co^{2+}, Hg^{2+}, Cu^{2+}, Fe^{3+} through monitoring photoluminescent features. We found that the fluorescence property of Au NCs shows four different behaviour like enhancement, equivalence, decrement, and quenching in accordance with the kinds of metal ions. In particular case, we also found that the altered fluorescence intensity of Au NCs was recovered after the addition of EDTA, which can abstract metal ion. Additionally, we will further mechanistic study for the change in the optical behaviour of Au NCs depending on metal ions.

Poster Presentation : **ANAL.P-265**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Characteristics and Electrochemical Performance of Silicon/Carbon nanofibers/Graphene Composite films as Anode Material for Binder-Free Lithium ion Secondary Batteries

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We report the interfacial study of a Silicon/Carbon nanofiber/Graphene Composite material as a potentially high performance anode for rechargeable lithium ion batteries. Carbon Nanofibers (CNFs) were grown using an iron-copper catalysts by the Chemical Vapor Deposition method. Silicon nanoparticles (SiNPs)/Carbon nanofibers (CNFs)/reduced Graphene oxide (rGO) composite films were prepared by simple physical filtration and an environmentally friendly thermal reduction treatment. The films were used as a high performance anode material for self-supporting, binder-free lithium ion batteries. The Silicon nanoparticles were uniformly coated with thermally reduced Graphene oxide (rGO), carbon nanofibers are wound round the surface of the graphene-coated silicon nanoparticles. Reducing graphene oxide has the effect of improving electron conductivity and accommodating volume change during repeated charge/discharge processes. Carbon nanofibers can help maintain structural stability and prevent detachment of silicon nanoparticles from the electrodes. When the produced Si:CNFs/rGO=1:1 composite films was used as an anode of a lithium ion batteries, the initial specific capacity was measured to be 1,894.54 mAh/g at a current density of 0.1 A•g^{-1}. After 100 cycles, the reversible specific capacity can be remained at 964.68 mAh/g, the coulombic efficiency can be reached to 93.8% at the same current density. In addition, the SiNPs/CNFs/rGO composite films electrode exhibited a better high specific capacity and cycle stability than an SiNPs/rGO composite films electrode (the reversible specific capacity is 277.28 mAh/g after 100 cycles), the Si:CNFs/rGO=3:2 electrodes (the reversible specific capacity is 545.9 mAh/g after 100 cycles) and the Si:CNFs/rGO=2:3 electrode (the reversible specific capacity is 462.9 mAh/g after 100 cycles). The SiNPs/CNFs/rGO composite films can effectively accommodate and buffer changes of silicon volume, form a stable Solid Electrolyte Interface (SEI), improve the conductivity of the electrode

and provide a fast and efficient channel for electron conduction and ion transport. This technology shows a great promise for the application of anode materials in the field of lithium ion batteries.

Poster Presentation : **ANAL.P-266**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Development of analysis methods for the toxic chemicals in Consumer Chemical Products (CCPs)

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Consumer Chemical Products (CCPs) provide enormous benefits to people, which make them indispensable part of modern life. However, there reported numerous chemical incidents regarding to CCPs represented by incident of disinfectants for household humidifiers in Korea. For the prevention of these chemical incidents, the Ministry of Environment have begun to regulate the chemicals in the CCPs, and the toxicity evaluation of CCPs have become the important issue. Effect-directed analysis (EDA) is one of the promising tool for the identification and evaluation of toxicants, which is combination of multiple procedures such as toxicity testing, fractionation, chemical analysis, and identification of toxicants. In this research, as the preliminary step, we developed analysis methods (HPLC, GC-MS, and LC-MS) to determine the concentration of chemicals for the nine chemicals in five CCPs (among detergent, bleach, deodorizer, and adhesive).

Poster Presentation : **ANAL.P-267**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

New named "Spectrator" as a device for the determination of titration end-points

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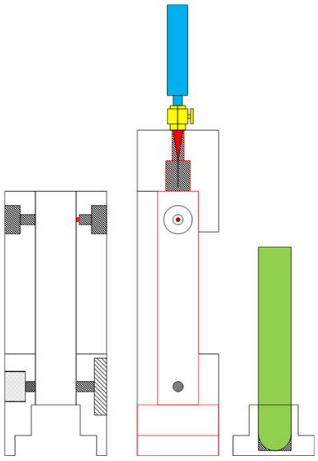
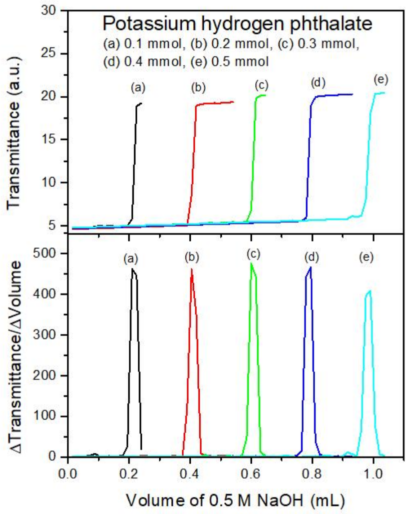
Division of Life Science and Chemistry, Daejin University, Korea

Many chemical reactions on a titration are including the change of not only potentials but also colors. In a potentiometric titration, it is obtained as a titration curve by measuring the abrupt change of the potential at the end-point. An acid-base titration is generally done by observing the color change caused by an indicator to determine the end-point. The method of determining the end-point by measuring the potential difference has been well established and commercialized, but there are not many devices that obtain the end-point by observing the change in color. A simple and precise spectral end-point detector can be manufactured by using a drop-counter consisted of IR-LED and –detector, a white light LED as the light source and a photo-detector, and an AD-converter(Arduino). Spectrator showed excellent results in terms of the reproducibility in acid-base titration using an indicator and in iodometric titration without an indicator. We intend to share the results of the Spectrator manufacturing process and the experiment using it.




Potassium hydrogen phthalate
(a) 0.1 mmol, (b) 0.2 mmol, (c) 0.3 mmol,
(d) 0.4 mmol, (e) 0.5 mmol
(a)
(b)
(c)
(d)
(e)
Transmittance (a.u.)
30
25
20
15
10
5
ΔTransmittance/ΔVolume
500
400
300
200
100
0
0.0
0.2
0.4
0.6
0.8
1.0
Volume of 0.5 M NaOH (mL)

Poster Presentation : **ANAL.P-268**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Kinetic modulation of Amyloid-β through its point mutation by structure-based design

Dongjoon Im, Chae Eun Heo, MyungKook Son, Chae Ri Park, Sooyeon Chae, Min Ji Kim[1], Hugh I. Kim*

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Modulating the formation process of amyloid-β fibril, especially kinetically delaying its early onset, is an applicable solution for Alzheimer's disease patients along with early diagnosis. The aggregates of Amyloid-β (Aβ) fibrils which are commonly observed in the brain of the Alzheimer's disease patients are considered to be closely related to the pathogenesis of the disease. Amyloid-β peptides with different number of residues may look alike but clearly have different physical properties. The peptides consisting of 40 and 42 amino acids, the two most dominant species, only differ in two amino acids of the N-terminal which is what provokes the difference of the entire morphology of their fibril structure, accelerated fibrillation of Aβ 42 to Aβ 40 as well as other properties. Since Aβ 42 to Aβ 40 ratio is found to be higher in patients compared to non-patients, we suggested the distinct physical properties of Aβ 42 to act as key factors in making it prone to self-assembly. In this study, we rationally designed mutant peptides with various point mutations based on their structure and physical properties. Designed mutant peptides have not only shown suppressed self-assembly, but also slowed down fibrillation process when mixed with wild type Amyloid-β (1-42).

Poster Presentation : **ANAL.P-269**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Serum exosomes analysis differentiating patients of alcoholic and nonalcoholic fatty liver diseases

Huu-Quang Nguyen, Jaebeom Lee, Jeongkwon Kim*

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Exosomes contain many biological materials originated from the releasing cells, including proteins, lipids and RNAs, and are known to be involved in the communication and transferring of components between cells.

In this study, exosomes were enriched from blood serum of patients diagnosed with various states of liver diseases, using multiple centrifugation cycles at 40,000 x g. The enriched exosome samples were analyzed using liquid chromatography tandem mass spectrometry (LC-MS/MS) with Orbitrap mass analyzer. The proteomics data from Orbitrap LC-MS/MS measurements were quantified using MaxQuant software with label-free quantification workflow, followed by univariate and multivariate statistical analysis. By analyzing 24 samples of four different liver disease types, significant differences in protein expression between the diseases, including previously reported markers of liver diseases. Principal component analysis using significantly altered proteins identified from MaxQuant analysis of the LC-MS/MS data provided a confident differentiation between alcoholic and non-alcoholic fatty liver disease groups.

These results provide insight into the use of exosome analysis using mass spectrometry-based proteomics as a tool to assist in diagnosis and prognosis in clinical settings. The new findings open up new possibilities of using mass spectrometry for point-of-care clinical applications as well as for disease discovery and prevention purposes.

Poster Presentation : **ANAL.P-270**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Structural studies of antimicrobial peptides derived from bovine milk with enhanced antimicrobial activity using NMR spectroscopy

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As antibiotic resistance increases, antimicrobial peptides (AMPs) studies have become important. However, due to their advantages, there is still the potential for being used as candidate of good antimicrobial agent. So we study LPcin-I and LPcin-II derived from lactophoricin, a cationic amphipathic antimicrobial peptide consisting of 23 amino acids, corresponds to the carboxyl terminal 113-135 region of Component-3 of bovine proteose-peptone PP3. Here we found that antimicrobial activity in the polypeptide is related to the N-terminal and modified to enhance antibacterial activity using single/double amino acid substitutions, sequence shuffling for better amphipathic characteristics. Therefore, we design YK1, YK2 and YK3 derived from LPcin-I. And among these, we used YK3 to improve AMPs with a shorter length because it show the best antimicrobial activity. First, the serine located in the hydrophilic part was mutated into lysine to increase the net charge of peptide. Next, amphipathicity was reduced to prevent self-aggregation. Finally, tryptophan was added to facilitate interaction with the bacterial membrane. Therefore, we designed and confirmed the new antimicrobial peptides YK5, YK8 and YK11 based on YK3. Analog peptides were obtained with high yield and high purity by optimizing expression using E. coli and purification using many biophysical techniques. We analyzed structural studies of novel AMPs using MALDI-TOF MS and CD spectrometry as well as NMR. In order to investigate the structures and dynamics, we use various 1D and 2D NMR techniques using micelle and especially bicelle samples to mimic membrane environments. The structural calculations of LPcin analogs using Discovery Studio 3.1 and tilt angle prediction based on SAMPI4 Solid state NMR spectra.

Poster Presentation : **ANAL.P-271**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

NMR structural studies and anti-inflammatory effect of the expressed tIK peptides

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Rheumatoid arthritis begins with inflammation in the synovial membrane around the joint, destroying cartilage and ligaments, and can also spread to blood vessels and skin, causing vasculitis, anemia, and headaches. There are many causes for the disease, but one of them is known as the imbalance of pro-inflammatory cytokines and anti-inflammatory cytokines. Recent studies have showed that truncated-IK (tIK) protein down-regulate inflammatory cytokines. Therefore, we conducted a study to develop anti-inflammatory peptides based on tIK full-length. In tIK transgenic mice, macrophages were isolated and examined for phosphorylation patterns. As a result, tIK protein phosphorylated 496th tyrosine of interleukin (IL)-10 receptor subunit alpha and showed anti-inflammatory effect. To find specific regions of tIK proteins that induce IL-10 receptor phosphorylation, we predicted the structure of tIK and proposed four epitopes by sequence homology modeling. TH17 cell differentiation tests confirmed their anti-inflammatory activity, among which a peptide consisting of 18 amino acids with anti-inflammatory activity were named tIK 18-mer. Afterwards, we found 9-mer and 14-mer, based on 18-mer. Expression was performed successfully using E.coli and the purification processes were optimized. This was confirmed using MALDI-TOF and NMR spectra. The secondary structure of each protein was confirmed through studied through CD and 2D NMR. Also, chemical shift perturbations were studied to confirm the mechanism. Finally, the anti-inflammatory test was conducted once more with the expressed protein that was successfully purified to confirm the effect. Interestingly, the anti-inflammatory effect of the expressed peptides was much better than that of the synthesized peptide tIK-9mer.

Poster Presentation : **ANAL.P-272**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Preparation of radiolabeled microplastics for its *in vivo* behavior research

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The continuous release and breakdown of large plastic wastes as well as direct emissions result in an accumulation of microscopic plastics, so-called microplastics, in ecosystem. Microplastics are contaminants of emerging concern, especially in human, and the number of studies of the toxicity of microplastics is rapidly increasing. To assess the risk posed by toxicity to human health, it is essential to evaluate their behavior *in vivo*. We decided to use radioisotope tracing or imaging for analyzing *in vivo* behavior of microplastics, such as uptake, distribution, accumulation, excretion. For such studies, radiolabeling of microplastics is essential, and we report the synthesis of radiolabeling of PVC, the first microplastics we try to analyze. For PET and SPECT imaging and excretion studies, we want to label PVC with Cu-64 or Lu-177 that can be chelated with NODA. NODA-NH_2 was conjugated to carboxylic acid groups on the PVC-COOH. NODA-conjugated PVC was characterized by analytical techniques such as NMR and DLS(to determine the microplastics length). NODA-conjugated PVC was then labeled with ^{64}Cu($t_{1/2}$=12.7 hr) and ^{177}Lu($t_{1/2}$=6.73 days). The yield of ^{64}Cu and ^{177}Lu-labeled PVC were 75% and 98%, respectively. The PET or SPECT imaging studies and excretion evaluation using these radiolabeled microplastics are under progress.

Poster Presentation : **ANAL.P-273**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Infrared spectroscopic screening of gall bladder cancer using bile juice as a specimen

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Human bile plays on important role in digestion step and enterohepatic circulation. By these processes, cholesterol molecules are transported without aggregation and bilirubin and bile acids are circulating from liver to intestine. As bile is stored in gallbladder (GB), composition of bile is varied by health condition of each person. In this study, bile samples were obtained from 5 normal, 20 GB polyp, and 10 GB cancer subjects, each bile sample was separated into the aqueous, organic, and amphiphilic phases by chloroform and methanol. 3 μL of each separated sample was dropped on hydrophobic OTS (octadecyltetrachlorosilane)-coated Si wafer to form reproducible circular droplet and dried for IR spectral acquisition. When the principal component scores obtained from the sample IR spectra using principal component analysis (PCA) were employed for k-nearest neighbor (k-NN) for discriminant analysis, the identification accuracy for GB cancer was greater than 97.1%. Based on the composition analysis using LC-MS, the concentrations of conjugated bile acids and contents of phospholipid classes such as phosphatidylcholines and phosphatidylethanolamines were different in the GB cancer samples.

Poster Presentation : **ANAL.P-274**

Analytical Chemistry

Zoom 5 WED 17:00~17:30

Influence of the Preferred Orientation of Pyridine Derivatives with Donor Substituents on Chemical Interface Damping Induced in Silver-Coated Gold Nanorods with Different Shell Thicknesses

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Chemical interface damping (CID) is one of the plasmon decay processes caused by adsorbate molecules in gold nanoparticles. Despite the advances in this field, the effect of pyridine derivatives having a preferred orientation on CID in silver-coated gold nanorods (AuNRs@Ag, core@shell) with different shell thicknesses remains unknown. Herein, dark-field scattering studies using pyridine derivatives with donor substituents as adsorbates in single AuNRs@Ag with two different Ag shell thicknesses are described. Pyridine derivatives having electrondonating groups (EDGs) were adsorbed on single AuNRs@Ag and induced a strong CID through the interaction of nitrogen with the Ag surface. AuNRs@Ag with thick shells showed a considerably enhanced CID effect compared with AuNRs@Ag with thin shells for all pyridine derivatives. Furthermore, pyridine derivatives with EDGs in the para position (4-aminopyridine and 4-dimethylaminopyridine) caused a decrease in the localized surface plasmon resonance (LSPR) linewidth broadening of single AuNRs@Ag compared with unsubstituted pyridine under the same experimental conditions. In contrast to the high inclination of pyridine molecules, pyridine derivatives bearing EDGs adopted a parallel orientation to the Ag surface according to surface-enhanced Raman spectroscopy and dynamic light scattering measurements, which resulted in different surface coverage on the Ag surface and decreased LSPR linewidth broadening. Therefore, this study provides deeper understanding of the effects of pyridine derivatives with donor substituents and Ag shell thickness on CID in single AuNRs@Ag.

Poster Presentation : **ANAL.P-275**
Analytical Chemistry
Zoom 5 WED 17:00~17:30

Investigating the Structural and Functional Characteristics in Glycated Hemoglobin Using Ion-Mobility Mass Spectrometry

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Hemoglobin is the major oxygen-transport protein which is a tetramer consisting of four globin chains and non-protein prosthetic heme groups. Human red blood cell hemolysate contains several minor hemoglobin components and the most abundant one is Hemoglobin A1c(HbA1c) which is formed by reaction with glucose and hemoglobin. This post-translational modified protein is called glycated hemoglobin and it is widely used as one of the most reliable markers for monitoring long-term glucose control in diabetic patients. In this modification, the carbonyl group of glucose attaches to the N-terminal of residues to form a labile aldimine (Schiff's base), and rearranges to generate a more stable ketoamine via Amadori rearrangement. To investigate the functional characteristics of glycated hemoglobin, we compared the oxygen affinity for hemoglobin and glycated hemoglobin. Then, we identified its residues of glycation in hemoglobin by electrospray ionization mass spectrometry. Finally, we investigated the mechanism of oxygen kinetics through using various tools including ion-mobility mass spectrometry, circular dichroism, and small-angle X-ray scattering.

Poster Presentation : **ANAL.P-276**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

NMR spectroscopy applications in plant metabolomics

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Chemical accidents can cause various damages raging from human health, ecosystem and material damage. After the chemical accident, the method or procedure for estimating the damage amount for plant damage has not been established in detail, and the data for the plant damage test evaluation method are also insufficient. Therefore, it is necessary to establish specific damage estimation methods and procedures to estimate the economic loss of plant damage due to chemical accidents. This study aimed to contribute to the standardization of sample preparation methods for the application of solution-state NMR, HR-MAS NMR and solid-state NMR spectroscopy, and to prepare test evaluation methods and damage estimation methods for solid phase samples in the field of chemical accidents.Garlic and onion are the popular ingredients and spices in the world wide. Due to the geographical advantage, large quantities of Chinese garlic and onions are being imported into Korea. Since it is difficult to discriminate agricultural products' country of origin by appearance accurate and detailed analytical techniques should be introduced. NMR spectroscopy is widely used to study the metabolic variation because NMR spectra focused on minor ingredients as well as major chemical components. For an association between metabolite and climate in a study on the metabolic dependences on *Allium* variety, harvesting area, ^{1}H NMR spectroscopy based on metabolomics provides useful information. In this study, the various metabolites of garlic and onion were identified and the quantitative difference in metabolites with origins of growth and harvest using solution-state NMR, HR-MAS NMR and PCA.

Poster Presentation : **ANAL.P-277**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Structural studies of human transmembrane proteins related to disease

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Heparan sulfate proteoglycan (HSPG), Syndecans, participate in biologically important interactions such as cell-matrix, cell-to cell interactions. Syndecan-4 (Syd4) may affect tissue development and repair as well as the pathogenesis of numerous diseases (e.g. cancer). The transmembrane domain of syndecan-4 has dimer or oligomer formation that are crucial for transduction signals. We demonstrated optimized method for expression and purification of three kinds of wild type Syd4 (wt-Syd4), mutant Syd4 (m-Syd4), and Syd4-eTC. Syd4-eTC has extracellular, transmembrane and cytoplasmic domain of Syd4. Highly purified proteins through optimized experimental procedure were employed to various analysis techniques such as PAGE, CD, MS spectrometry, solution-state and solid-state NMR spectroscopy. In addition, we got ^{1}H-^{15}N 1D, 2D SAMMY and SAMPI spectra using home-built solid-state NMR probe.The transmembrane domain of amyloid precursor proteins (APP-TM) related Alzheimer is the multimer formation of amyloid beta channels that composed of several human amyloid beta (hAβ) monomer. APP-TM forms ion channel that Ca2+ permeability in the cell membrane and these channels can disrupt the normal cellular calcium homeostasis. Recently, various inhibitors of blockers such as zinc (II) ions of these ion channels are developed based on structural feature between amino acid and functional group of inhibitor. In case of the APP-TM, we demonstrated the three dimensional structure of the transmembrane region of APP-TM in the membrane using 1D/2D solution and solid-state NMR spectroscopy.

Poster Presentation : **ANAL.P-278**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Homologous recombination repair and cholesterol-mediated drug efflux induce dose-dependent chemoresistance in nutrient-deprived neuroblastoma

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Neuroblastoma is a solid pediatric tumor with heterogeneous clinical behaviors. Chemotherapy is widely used to treat neu-roblastoma; however, dose-dependent responses and chemoresistance mechanisms of neuroblastoma cells to anticancer drugs remain challenges in various conditions. Here, we investigated the dose-dependent effects of topotecan on human neuroblastoma cells (SK-N-SH, SH-SY5Y, and SK-N-BE) under various nutrient supply conditions. Serum-starved human neuroblastoma cells showed reduced toxicity, and their survival rate increased upon treatment with a high concentration (1 μM) of topotecan. Quantitative proteomics identified approximately 10,000 proteins in SK-N-SH cells. Network analysis revealed that topotecan up-regulated DNA repair and cholesterol-mediated topotecan efflux, resulting in topotecan re-sistance. Results of cell cycle and quantitative analyses of membrane cholesterol supported the validity of these resistance factors and their applicability to all neuroblastoma cells investigated in this study. Our results provide a model for high dose-dependent chemoresistance in neuroblastoma cells that could enable a patient-dependent chemotherapy screening strategy.

Poster Presentation : **ANAL.P-279**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Integration of Surface Enhanced Raman Spectroscopy with Polymerase Chain Reaction for Monitoring K. pneumoniae

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Surface enhanced Raman spectroscopy (SERS) is a technique that is widely used for the monitoring chemical and biological analytes due to its potential of multiplexing ability and sensitivity. More recently, it has been also used to analyze various disease-related nucleic acid biomarkers for the monitoring infectious disease and tumor. Even though its multiplexing ability, result-reproducibility is one of potential threat which makes difficulty of using in the field. Normally it happens according to the low target concentration within highly complex biological samples such as rare mutation and early stage infection status in patients. In this study, in order to improve the sensitivity of detection for monitoring nucleic acids, SERS was integrated with polymerase chain reaction (PCR) to amplify target-specific nucleic acid that triggers SERS amplification sequentially. Based on this, we attempted to develop a technology that capable to simultaneously detect various disease-related pathogens in a multiplexed and sensitive manner. To increase the sensitivity and selectivity of detection, silver and gold hybrid star-shaped nanoparticles (Au-Ag HNPs) were synthesized and nucleic acid Raman probe were immobilized on the Au-Ag HNPs. Basically PCR amplifies pathogen-specific SERS residues and amplified sequences trigger conformational change of target-specific Raman probes by complementary interaction. As a model system, primers and probes are designed against K. pneumoniae and PCR-based target sequence amplification were initiated SERS signal enhancement. We believe this platform technology can be used for monitoring rare-pathogen from complex biological samples such as blood and saliva in a multiplexed and sensitive manner.

Poster Presentation : **ANAL.P-280**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Tunable Chirality in Two Thumbs film

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Nature-mimmetic chiroptical metasurface has become a challenging flat optics research theme to apply stereochemistry, molecular biology, crystallography, and further secure quantum communications. In this article, chiral metasurfaces transferred from commercial optical grating were fabricated by using a polydimethylsiloxane (PDMS) film, in which the chirality of the metasurface film was readily tuned to be left- and right-handed by modulating the angle (θ) between the curvature vector and the grating direction, i.e., blaze arrow. Furthermore, a fingerprint – transferred PDMS metasurface with Au coating was prepared to investigate nature-induced chirality and surface plasmon resonance (SPR). Indeed, the fingerprint-transferred metasurface showed unique chiroptical SPR property, induing surface enhanced Raman scattering (SERS) effect to monitor chiral molecules. It is probably ascribed to the grating-like pattern and curvature of the PDMS film transferred the human thumb, similar to the as-designed grating. It is probable that these results will open a novel approach to produce facile chiral metasurfaces.

Poster Presentation : **ANAL.P-281**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Evaluation of weighted ensemble Twin support vector machine for near-infrared spectroscopic discriminant analysis

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Weight ensemble TW-SVM (we-TW-SVM) has been proposed as potential multivariate chemometric classification method for NIR spectroscopic identification of geographical origins of agricultural samples. NIR spectral features of individual components in a sample are broad and extensively overlapping with each other since they are originated from overtone and combination vibrations. To recognize minutely different spectral features present over a whole spectral range, twin SVM (TW-SVM), which utilizes two non-parallel hyperplanes built simultaneously for better identification of one class and maximization of distance from other classes, was previously proposed. Further, in this study, we-TW-SVM combining the weights that minimize prediction errors has been proposed. First, the weights are trained to minimize the difference between the actual geographical origin of the sample and the predicted geographical origin by TW-SVM. As a result, the weighted spectrum highlights the characteristics of the agricultural product's geographic origin. Second, a hierarchical ensemble technique is applied to create robust model that gives stable discrimination accuracy for various data types. To evaluate the potential utility of we-TW-SVM, NIR spectroscopic discriminations of the geographical origins of the 19 agricultural products (adlay, adzuki, black soybean, green kernel black bean, garlic, glutinous foxtail millet, jujube, lingzhi, mung, milk vetch root, omija, panicum, peanut, pepper, pine nut, sesame, shiitake, sorghum, white soybean) were performed using SVM, TW-SVM, and we-TW-SVM, and resulting discrimination accuracies were compared with each other.

Poster Presentation : **ANAL.P-282**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

An integrated approach for probing quaternary structure change of protein induced by ligand using SAXS and cross-linking/MS

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Characterization of the protein-protein interactions is crucial for the study of a wide variety of biological systems. Numerous research has been reported that various methods are developed to support the identification, characterization, and analysis of protein complexes. Since the protein-protein interactions are easily influenced by post-translational modification (PTM), metal ions, and ion concentration, the development of methods to probe protein-protein interaction induced by environmental factors is needed. Here, we have investigated the ATP effect on the quaternary structure of insulin using multiple biophysical analyses. Firstly, we have conducted the solution small-angle X-ray scattering (SAXS) experiments to understand insulin overall size information, protein association state from their scattering profiles. Then, to identify, characterize, and quantify intermolecular protein-protein interactions in the presence and absence of ATP, we performed crosslinking-mass spectrometry (XL-MS) using two crosslinkers. Finally, we executed molecular docking simulation using our obtained information from the XL-MS regarding residue-residue interaction, and simulated structures were compared to the experimental SAXS profiles to suggest possible protein structures. The experimental methodology using diverse analytical techniques would be highly helpful in understanding the protein-protein interactions.

Poster Presentation : **ANAL.P-283**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Comparison of Fibrillation Kinetics of Amyloid Proteins in H2O and D2O

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Heavy water, D2O, has been used in Infra-Red (IR) spectroscopy, Nuclear Magnetic Resonance (NMR), etc., to avoid the interference of O-H frequencies and H resonance frequency when light water, H2O is used. Specifically for IR, amide I band of peptides and proteins is 1600-1700 cm-1, while the H2O vibrational frequency is 1643.5 cm-1 overlapping the amide I band. Also, hydrogen-deuterium exchange (HDX) mass spectrometry is utilized to study protein tertiary structures.But since D2O is more polar than that of H2O, the hydrophobic effect of D2O is also stronger. So, the properties of the protein in H2O and D2O for example, protein stability, can be different. Efimova et al., have compared the stability of globular protein, lysozyme and bovine serum albumin in H2O and D2O, using differential scanning calorimetry (DSC). Proteins were more stable in D2O, with a wider pH range of stable form of BSA. There are some similar studies, but little about the protein fibrillation in D2O is known. Hydrophobic interaction of proteins is significant to the fibrillation of amyloidogenic proteins and protein structures. In this study, we have compared the hydrophobic interactions, structures and stability of amyloidogenic proteins, insulin and alpha-synuclein, using various spectroscopic methods, Fourier transform IR (FT-IR) spectroscopy, 2D-IR spectroscopy, ion mobility mass spectrometry, small angle x-ray scattering, thioflavin-T assay, DSC, etc.

Poster Presentation : **ANAL.P-284**

Analytical Chemistry

Zoom 5 WED 17:30~18:00

Proteomic analysis of environmental stress in correlation with physiological changes in *Haliotis discus hannai*

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With its high market worth and nutrient value for humans, *Haliotis discus hannai*, also known as the Pacific abalone, is a valuable commercial fishery resource in eastern Asia. Various environmental factors, such as temperature, salinity, oxygen, and CO_2 influence its growth and development. Among them, temperature and salinity are the primary physical factors that are affecting the distribution and physiological metabolism of shellfish. These environmentally stressed shellfishes are highly susceptible to pathogens which increase the mortality rate in aquaculture systems. This study aims to determine the physiological changes in *H. discus hannai* by detecting the protein expression of *H. discus hannai* which is influenced by changes in water temperature and salinity. Proteins were extracted with RIPA buffer from homogenized hepatopancreas tissue of *H. discus hannai*. Each supernatant fluid was pooled into experimental and control groups according to the period of exposure to environmental stress. Pooled samples from *H. discus hannai* were trypsin digested and desalted. Subsequently, the proteins in each group were analyzed with nLC-MS/MS and by protein database searches, and then the effect of environmental stress was also determined with differentially expressed protein (DEP) and gene ontology (GO) enrichment analysis.

Poster Presentation : **ANAL.P-285**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Photothermal effect analysis of Bi-Te covered nanorods on 3D spheroid neuroblastoma cells

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Neuroblastoma is a solid tumor that almost always affects children. It starts in immature nerve cells found in an embryo or fetus. These days, nanoparticle for cancer treatment is being actively studied. The major function of these nanoparticles in therapy is drug delivery vesicles, imaging agents, and photothermal effect etc. So far, most studies of nanoparticle have been based on two-dimensional (2D) cell models. However, 2D cell models are hard to provide an accurate representation of the in vivo environment of the solid tumor. In this study, we use three-dimensional (3D) human neuroblastoma SK-N-SH cell spheroid models instead of 2D cell models to overcome the limitation of 2D cell models. After 5 days of culturing 3D spheroids, we treated Bi-Te covered nanorods (BTCN) that is previously reported for its photothermal and photoacoustic effect on 2D cancer cell models. BTCN is dissolved in serum free media and treated at spheroids with various concentrations for 4 hours. Then, 808nm 5 W/cm2 near IR laser light is irradiated for 2 minutes per one spheroid. After this process, we measured cell viability of the spheroids to identify the effect of BTCN with laser irradiation in 3D cell models. Also, we examine a form of the spheroids through a microscope, looked at the distribution of living cells and dead cells through confocal microscope. The results obtained from these techniques will help us to find out the difference between the therapeutic effects of BTCN in the 2D and 3D cell models, and how to increase their effectiveness in 3D cell models that is similar to reality.

Poster Presentation : **ANAL.P-286**

Analytical Chemistry

Zoom 5 WED 17:30~18:00

Turbidity measurement in absorbance unit

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Turbidity refers to the cloudiness of water which loses its transparency by suspended particulate mattes and is used as an good indicator of water pollution level. Turbidity is commonly measured in NTU (Nephelometric turbidity unit). This method is not a direct measure of suspended particles in water but, instead, a measure of light intensity which is scattered by particles at an right angle. IR wavelengths is widely used for this purpose. Absorbance unit also can be used to measure the turbidity. Turbidity measured in NTU usually shows lower precision and accuracy at low levels in turbidity below ~10 NTU compared to the turbidity measurement in absorbance unit. In this study, a commercially available low cost turbidimeter was purchased and modified to measure a turbidity of the same turbid sample with both NTU and absorbance unit at the same time. This modification was done to compare both turbidity measurement methods and then which method is more effective for a certain condition (i.e. the degree of turbidity, linearity, type or color of suspended particles and so on). The calibration curve for the 1-400 NTU range showed R2=0.9996 in NTU unit and R2=0.9978 in absorbance unit respectively. So the linear range and linearity is almost same but absorbance unit showed overall better precision. This study shows that using ratiometry can improve the precision in turbidity measurement in NTU unit also. Furthermore, absorbance unit reflected the clarity of water more accurately which contained suspended black particles. The black particles even reduced the overall turbidity in NTU unit when the black particles was added to the turbid sample with suspended white particles. At a concentration of 1NTU, %RSD of turbidity meter decreased from 22.9% before calibration to 11.8% after calibration, and absorbance decreased from 24.5% before calibration to 2.7% after calibration. In the charcoal and turbidity sample mixture, the turbidity measurement decreases and the absorbance measurement increases. And we checked the effect of charcoal on turbidity by mixing the turbidity standard solution and charcoal. a photodiode measuring 890nm LED's reference and absorbance was attached to the turbidity meter sold on the market, and a turbidity meter equipped with the technology to measure correct turbidity and absorbance at the same time using the same sample was produced and evaluated., resulting in a disadvantage of having to produce a calibration curve each time for accurate measurements. Therefore, effective calibration techniques are needed to improve accuracy for low concentrations of turbidity measurements.

Poster Presentation : **ANAL.P-287**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Combining Clinical Implications from TCGA GBM and Proteomic analysis of IDH1 mutated cell-line to investigate the role of IDH1 mutation in GBM

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Glioblastoma multiform (GBM), is an aggressive type of cancer that occurs in the brain or spinal cord. A recent genome-wide mutational analysis revealed IDH1 mutation, a common mutation found in GBM, to be associated with the increase in overall survival of GBM patients. Despite its importance, proteome research related with IDH1 mutation has not yet been systematically reported. Interestingly, the construction of the IDH1 R132H point mutated cell-line showed morphological difference over distinct time periods suggesting IDH1 mutation playing dynamic roles in the progression of GBM.Comprehensive proteome profiling was performed for three replicate sets of 6-plex TMT, labeled with wild type(WT), day1(D1) and day 6(D6) samples of two successfully built IDH1 R132H mutated U87MG cell-lines (MT9-6 and MT9-19). IMAC enrichment was conducted prior to phosphopeptide profiling with our DO-NCFC-RP/RP-MS/MS platform, resulting in average 41,603 phosphorylation sites and 51,595 distinct phosphopeptides, corresponding to 7,352 protein groups. Global profiling from DO-RPLC-MS/MS analysis resulted in 259,061 distinct peptides which correspond to 11,868 protein groups (≥2 hits), and from our results, gene ontology enrichment analysis was carried out to investigate the early and late responses of the mutation.To add clinical implication to our proteomic data, gene signatures where identified from The Cancer Genome Atlas(TCGA) GBM data, confirming the four subtypes stated in a previous study (Cancer Cell 2010). Combining clinical gene signature data and our comprehensive profiling results, we plan to construct a network model associated with collagen, which are one of the geneset that showed high correlation between clinical and protein data, expecting to find hints in the role of IDH1 mutation and its application for GBM treatment.

Poster Presentation : **ANAL.P-288**

Analytical Chemistry

Zoom 5 WED 17:30~18:00

One-pot synthesis of water-soluble Iron Selenide Quantum Dots with chiral stabilizer

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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. Reaction was optimized by controlling reaction pH, time and temperature to improve the quantum yield. Transmission electron microscopy analysis suggests that the sized of FeSe QDs are distributed in the range of ~3.0-4.0 nm with a lattice spacing of 0.297nm. 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-289**

Analytical Chemistry

Zoom 5 WED 17:30~18:00

Colorimetric Strain Sensor by Magnetoplasmonic photonic crystal array on flexible substrate

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Recently, many people have challenged wearable devices. Wearable devices need to be able to constantly exchange information with users through sensors. Sensors used for the purpose of detecting various conditions output information in many cases as electrical signals. Signals transmitted as electrical signals have many advantages, but the need for low power, flexible sensors for long time use is increasing. The plasmonic noble metal is also used in color change papers using nanoparticles. These particles form a chain structure, form a plasmon coupling, and have a plasmon resonance on the surface. The reflectance of the surface changes by physical force, which is used for color sensors. In the papers describing the color change using nanoparticles, most use plasmonic noble metal as a particle. Plasmonic noble metal particles form a plasmon coupling forming a chain structure and has plasmon resonance on the surface. The reflectance of the surface is changed by physical force, and this characteristic is used in color sensors. For example, Au noble metal colloidal nanoparticles can be seen using plasmon resonance characteristics to show a change in color. In addition, Plasmonic microgel is magnified with temperature and color changes, so it is observed that the saturation changes with the temperature appear. Ag@Fe3O4 a film sensor using nanoparticles can visually represent a physical change and apply it to various movements. In addition, the advantage of being able to change the color of the sensor depending on the size of the nanoparticles will be used in a wide range during the actual application. In this paper, only physical reactions will show that the color changes without current and explain the principle. This will be able to achieve the purpose as a sensor by showing a definite change that differs from the saturation or brightness. To solve this problem, this paper attempts to fabricate a low-power, flexible physical sensor using photonic crystals and to verify the results of various experiments.

Poster Presentation : **ANAL.P-290**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

DO-NCFC-RP/RPLC combined with FAIMS for comprehensive proteomics analysis

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Human proteome analysis covering 10,000 proteins from a single cell type is possible, even if some methodological and technical problems remain. Identifying more than 10,000 proteins is still significant challenge, because identification efficiencies of present technology decrease under this condition. In this study, we introduce a dual online reverse-phase/reverse-phase liquid chromatography system based on an online non-contiguous fractionating and concatenating device (NCFC fractionator). In proteome analysis of complex human proteome, this system offers improved exploitation of separation space, so that a significant increase in the number of proteins identified in comparison with a common contiguous 2D-RP/RPLC method. In addition, the perfectly automated DO-NCFC-RP/RPLC system omits manual processes. As a result, this system minimizes sample loss and enables highly reproducible 2D-RP/RPLC experiments. Despite the advance in technology, a single-shot data dependent acquisition (DDA) is still limited to detection of complex human proteome. To increase the identification, we apply high-field asymmetric waveform ion mobility spectrometry (FAIMS) interface, which separate ions through differences in an ion's mobility at low and high electric fields between inner and outer electrode. This interface selects ions pass from the ion source to the mass spectrometer for improved selectivity improved detection limits, and increased throughput. Here, we will discuss comparison between DDA data and FAIMS data.

Poster Presentation : **ANAL.P-291**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Synthesis, Properties and Electrochemical Characteristics of SiNPs/CNT/rGO Composite films for Anode Material of Li ion Batteries.

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We have synthesized Silicon nanoparticles(SiNPs)/Carbon nanotubes(CNT)/reduced Graphene Oxide(rGO) composite films by facile dispersing technique and physical filtration and applied these composite films as a high performance anode material for self-supporting, binder-free Li ion batteries. The silicon nanoparticles were uniformly coated with thermally reduced graphene oxide and carbon nanotubes are wound round the surface of the graphene-coated silicon nanoparticles. Reduced graphene oxide provides matrix with enough void space to accommodate the volume changes of SiNPs upon lithiation/delithiation and simultaneously improve electron conductivity. Carbon nanotubes can also help maintain structural stability and prevent detachment of silicon nanoparticles from the electrodes. The thickness of composite films was controlled to 20ml, 25ml, 30ml respectively and electrochemical performances were compared each other. We have then characterized these composite films by scanning electron microscope, X-ray diffraction, transmission electron microscope, X-ray photoelectron spectroscopy, thermogravimetric analysis, and investigated the electrochemical properties by galvanostatic charge-discharge. The SiNPs/CNT/rGO composite film electrode exhibited a better specific capacity and cycle stability than the rGO/SiNPs composite film electrode.

Poster Presentation : **ANAL.P-292**
Analytical Chemistry
Zoom 5 WED 17:30~18:00

Limit of Detection for HPLC-Photodiode Array Detection is Comparable to the Refractive Index Detection for Monosaccharide Analysis.

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High-performance liquid chromatography (HPLC) is most commonly equipped with an ultraviolet (UV) absorbance detectors due to its easy-to-use and good stability qualities. One of the greatest limitations, however, is their failure to produce proper sensitivity for analytes missing a suitable UV chromophore. Refractive Index (RI) detection is indeed an alternate solution to satisfy the former's drawback, while knowing its limitation of using only the isocratic system for HPLC application. UV-absorbance detectors are often overlooked in sugar-related research due to the compounds' low to non-existent UV absorption. However, there is a crucial need to use the gradient method for sugar analysis, since each compound has a unique elution time. In this analysis, we compared the two detection methods for small sugars, i.e. fructose, glucose, sucrose and maltose, to determine the detection limit (LOD). Using the shortest wavelength (190 nm) of our photodiode array detector, the small sugars can be detected. We took this advantage to compare the LOD of the two detection methods, and our preliminary results suggest that the two are comparable for the monosaccharide analysis. This finding shows that UV-absorbance detection can be extended to monosaccharide quantification for quality assurance purposes.

Poster Presentation : **LIFE.P-293**

Life Chemistry

Zoom 7 WED 17:30~18:00

Divalent ionic regulation for co-formation of an actin-microtubule in vitro

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Actin and microtubules are main components of cytoskeleton, which are responsible for the cellular shape and motility through their dynamic interaction with their own unique morphological features. Although there are many known coupling proteins responsible for bridging actin and microtubules, little has been known how actin filaments and microtubules interact in a confined space while they are assembling. In order to understand the interaction between the two fibrils in the process of formation, the co-formation of actin-microtubules without any coupling protein was studied. Also, our team conducted research on the co-formation for actin-microtubules by regulating the concentration of divalent ions. We can compare those with the interaction mechanism, for example, the physical barrier mechanism and "cooperation of membrane protrusion" mechanism, in the absence of the binding protein. We have confirmed how actin acts as a barrier to the growth of microtubules. It has also been confirmed that actin filaments, by surrounding the microtubules, can participate in the "cooperation of membrane protrusion" mechanism. We also report the results of our research on the properties in vitro of and the conditions for controlling actin production, microtubule production, and actin-microtubule co-production through divalent ions.

Poster Presentation : **LIFE.P-294**

Life Chemistry

Zoom 7 WED 17:30~18:00

Artificial cellular model for morphological changes and motions with controlled actin polymerization

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In a cellular system, both the cytoskeleton and the membranes are under dynamic and complex networks to maintain its bioactivity. Generally, most of the researchers defined the general functions and bioactivities of these bio-compartments through *in vitro* experiments. However, *in vitro* experiments are limited to understand the interactions and dynamic networks between the compartments in a *cellular shape closed system*. Furthermore, as several researchers continuously found differences between *in vitro* and *closed system* experiments, the researchers are developing the *optimal closed system* for further understanding the cellular bioactivities. Here, we designed and built an **artificial cellular model** that explains the several different networks between differently conditioned membranes and self-polymerizing cytoskeletal proteins (F-actin). The GUVs had Mg^{2+} ionophores embedded, which enables Mg^{2+} to travel the inner condition of this model, which triggers the polymerization. As the cytoskeletal filaments grew in the GUVs, they protruded into the plasma membranes. The morphologies were different by the modified phase properties of the GUVs: ordered/disordered phases from saturated/unsaturated, charged/zwitterionic, or cholesterol-free/cholesterol-containing phospholipids. The morphologies are divided into three conditions, no interactions, interactions, and the creation of an inner crust. Our models are the *cellular shape closed system*, which shows the possibility of creating cellular morphological changes or motions with only the interactions between cytoskeletal proteins and membranes with controlled actin polymerization.

Poster Presentation : **LIFE.P-295**

Life Chemistry

Zoom 7 WED 17:30~18:00

Evaluation of the expression stability on housekeeping genes from Long-tailed chickens

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The real-time polymerase chain reaction (RT-qPCR) uses a housekeeping gene expressed as a reference gene in cells of all organisms, which measures the expression of PCR product amplified in real-time. However, since the expression of housekeeping genes can be affected by various conditions, it is important to select the optimal reference gene by exploring the housekeeping genes with high stability under condition. The current study analyzed the stability of the expression of six housekeeping genes (B2M, SDHA, GAPDH, RPL13, VIM and ACTB) in the tissues (heart, thigh and breast) of long-tailed chickens using Excel-based software tools, BestKeeper, geNorm, and NormFinder. The evaluation of the expression stability on housekeeping genes in RT-qPCR can be applied for accurate data analysis.

Poster Presentation : **LIFE.P-296**

Life Chemistry

Zoom 7 WED 17:30~18:00

Biochemical characterization of Glucose 6-Phosphate dehydrogenase from *Helicobacter pylori*

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Glucose-6-phosphate dehydrogenase catalyzes the oxidation of Glucose-6-phosphate to 6-Phosphogluconolactone. This is a part of the pentose phosphate pathway, and it is very important to understand the structure and kinetic parameters of *Helicobacter pylori* G6PDH(HpG6PDH) because NADPH, an essential cofactor, is produced. In this study, G6PDH of *Helicobacter pylori* was overexpressed in *Escherichia coli* and homogeneously purified for molecular and biochemical characterization. HpG6PDH showed activity to both cofactors, NAD^+ and $NADP^+$, and kinetic parameters for the substrates glucose6-phosphate, NAD^+ and $NADP^+$ were studied. The MALS results of HpG6PDH showed the formation of dimers. In the CD analysis, HpG6PDH showed a spectrum of an α/β structure, and melting temperature was measured from the thermal denaturation experiment. The molecular and biochemical features discovered in this study are expected to provide a basis for application in medical purposes.

Poster Presentation : **LIFE.P-297**
Life Chemistry
Zoom 7 WED 17:30~18:00

Cell Lysate-based Cell Free Expression in a giant liposome

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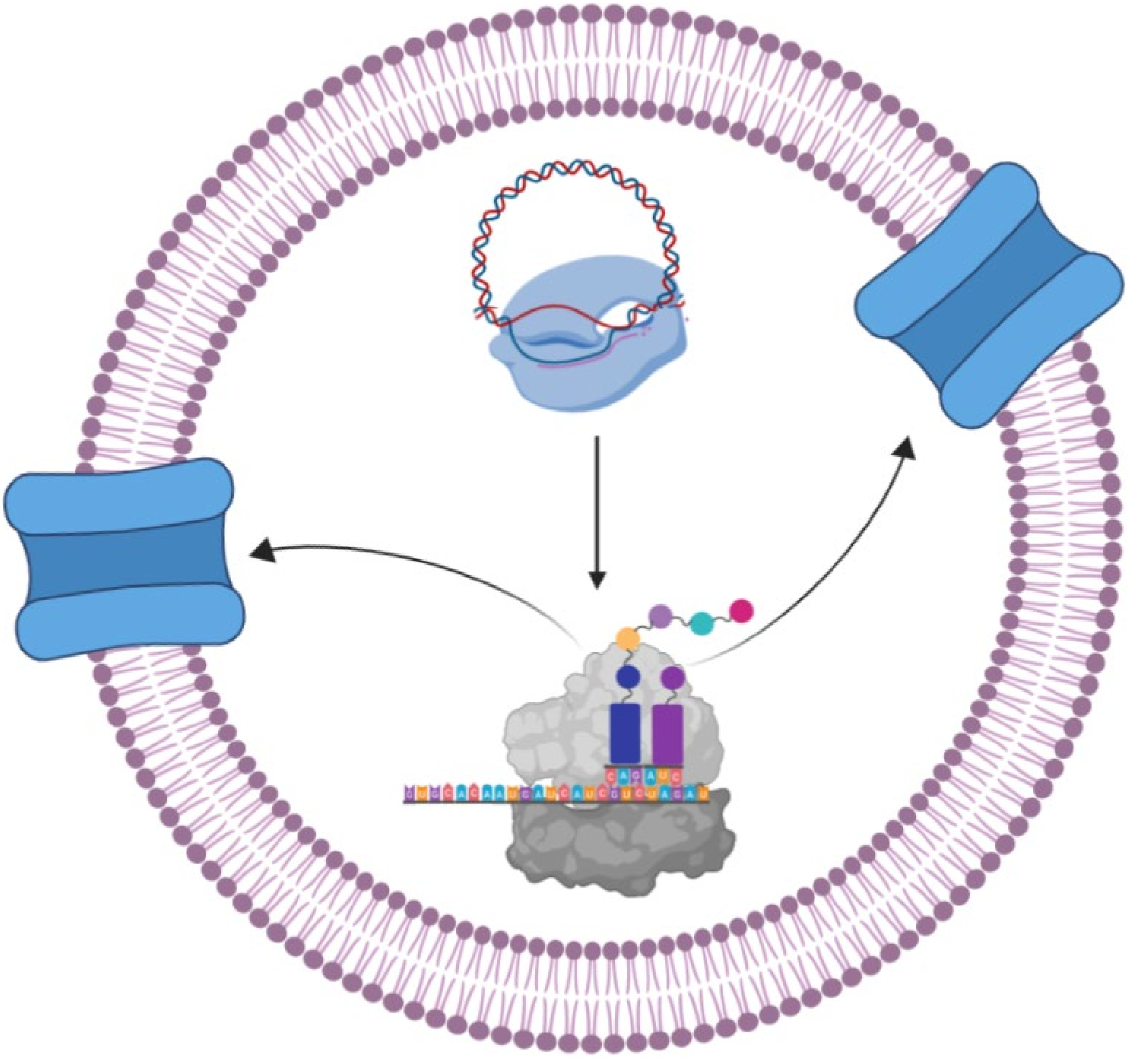
Cell-free protein synthesis (CFPS) which allows direct control of expression is one of the most promising models in the field of bottom-up synthetic biology. In particular, CFPS in giant unilamellar vesicle (GUV) has been being studied to make cell-mimicking artificial cells, and protein synthesis using recombinant elements (PURE) has been widely used as an optimized common reagent for protein expression. CFPS based on cell lysates, however, has not been studied well despite its tremendous potential functions originated from living cells, particularly in a vesicle, due to its difficulties in optimization and osmotic instability. Herein, with cell lysate-based CFPS system, we optimized the expression amount of proteins and adopted emulsion transfer method for preparing GUV with super high encapsulation efficiency. After that, we investigated phase separation of lipids and homogeneity of buffer, to stabilize the protein synthesis against osmotic pressure and maximize the expression ratio, respectively. With this widely applicable tool for bottom up synthesis, we are aiming to synthesize functional membrane proteins that would be integrated into the membrane of GUV and functioning from the cell lysate encapsulated in a GUV. In this fashion, with functional membrane proteins, signals from the outside would be delivered to GUV, and subsequently various biological reactions, designed with cell lysate-based CFPS can be triggered. We will present several protein synthesis processes in a single vesicle, designed, and controlled with cell lysates from bacteria.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Poster Presentation : **LIFE.P-298**
Life Chemistry
Zoom 7 WED 17:30~18:00

Collagen Fibrils Formation from Collagen-encapsulated Nanoliposomes using Electrical Stimulation

Albertus Ivan Brilian, Agustina Setiawati[1], ChangHo Kim, Kwanwoo Shin[*]

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Collagen is one of the prominent scaffolding components of the extracellular matrix that can turn into collagen fibers through self-assembly mechanisms. Recently, we found that the collagen fiber formation process can be stimulated by an electric field in an acidic condition through the aggregation of tropocollagen. Therefore, we designed an experiment to form collagen fibers by encapsulating collagen molecules in nano-sized liposomes (Lip-Col) and confirmed that the fibril could be formed from Lip-Col under an electric field in an acidic microenvironment. First, we measured the average particle size, encapsulation efficiency, and stability of Lip-Cols at various pH conditions. When applying an AC of 10Hz-1V, collagen fibers were appeared within ca. 20 minutes. Fluorescence imaging results showed that after applying an electric current for 2 hours, the collagen fibrils were formed in a matrix-like structure at pH 3, while they were in an aggregated form at pH 2. Based on these results, these Lip-Cols can be utilized as a drug delivery system for anti-aging or wound healing agents.keywords: collagen fiber, collagen fibril, liposome, electric field

Poster Presentation : **LIFE.P-299**
Life Chemistry
Zoom 7 WED 17:30~18:00

Development of modified spytag and spycatcher pair for application in affinity chromatography

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The SpyTag and SpyCatcher system is an efficient tool for bioconjugation of recombinant peptides. The SpyTag and SpyCatcher protein have relative high binding affinity (0.2 μM) and spontaneously form an isopeptide bond. Our research revolves around the application of this system in protein purification strategies employing affinity column chromatography. For this purpose, we aim to modify this system to prevent the formation of the irreversible isopeptide bond. To this end, we designed a mutated Catcher protein (K31R) which non-covalently binds to the Tag mostly relying on hydrophobic interactions. In an attempt to improve the binding affinity, we constructed the peptide libraries of the SpyTag. Based on the X-ray crystal structure, crucial amino acid residues were substituted for the more hydrophobic aromatic amino acids . At the same time, to ascertain the water solubility, non crucial amino acid residues were replaced by aspartic acid. The peptide libraries were constructed using solid phase peptide synthesis. Next, the binding of the on-bead peptide library to the fluorescent labeled Catcher protein was screened using a fluorescence microscope. In conclusion, Several modified Tag peptides were found to have improved binding with respect to the non-modified Tag peptide.

Poster Presentation : **LIFE.P-300**
Life Chemistry
Zoom 7 WED 17:30~18:00

Microwave-Assisted Solid Phase Peptide Synthesis (SPPS) for Cancer Diagnosis

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Recent advances in Proteogenomics analysis allows us to investigate the major causes of cancer by examining proteins and peptides of tumor tissue. However, it is still a complex and time-consuming process to determine exact characteristics of a given cancer, which makes difficult a fast and appropriate treatment of the cancer. To solve this issue, we have designed peptide templates composed of various isotope-labeled signal peptides, which are considered to be related to the tumor development. Through the isotope-labeled peptide templates and their mass spectrometry analysis, the database of tumor-associated peptides is being constructed, which we expect to contribute to reducing the diagnosis time for cancer. In this research, a library of labelled peptides has been synthesized by using microwave-assisted solid phase peptide synthesis (SPPS) and subsequent screening process. Microwave-assisted SPPS is composed of alternating Fmoc-deprotection/amide coupling reaction on the surface of PS substrate, which is accelerated with the help of microwave. The reaction variables such as reactant concentration, microwave power, etc. were adjusted to optimize the reaction process. After the synthesis of designed peptide linkage, the peptide was purified using HPLC. LC/MS/MS was used to characterize the molecular weight and linkage sequences of the synthesized peptide.

Poster Presentation : **LIFE.P-301**
Life Chemistry
Zoom 7 WED 17:30~18:00

DH002 stimulates glucose uptake in C2C12 and 3T3-L1 cells via inhibition of protein tyrosine phosphatases

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Type 2 diabetes mellitus (T2DM) is a disease characterized by insulin resistance. Insulin resistance has a feature of defects in insulin signaling and several protein tyrosine phosphatases (PTPs) involved in this signaling pathway can be potential antidiabetic targets. We have screened natural compound to identify potent inhibitors of PTPs involved in insulin resistance. Among them, DH002 inhibits several PTPs. Then, we examined its IC50 and cooperative binding through evaluating hill coefficient in vitro. In C2C12 myotubes and 3T3-L1 adipocytes, DH002 increased GLUT4 translocation to the plasma membrane protein and stimulates glucose uptake in a concentration-dependent manner. In addition, we demonstrated that DH002 stimulated glucose uptake through activation of AMPK and Akt signaling pathways. Thus, these results suggest DH002 as a potential therapeutic candidate for T2DM.

Poster Presentation : **LIFE.P-302**

Life Chemistry

Zoom 7 WED 17:30~18:00

JS-003 as a novel palliative natural compound of type 2 diabetes via downregulation of diabetes-related phosphatases.

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In recent society, many people have suffered from diabetes which is representative of chronicle diseases consist of two types: Type 1 diabetes and Type 2 diabetes. In terms of type 2 diabetes, It stems from the disability of glucose-uptake in cells related to insulin receptors as well as glucose transporters. Cell signalings induced by interaction between phosphorylation and dephosphorylation have a strong effect on expressing and translocation of these receptors and transporters. In this aspect, phosphatases play a significant role in type 2 diabetes mellitus. PTP1B, PTP-MEG2, SHP2, PTPRS, PTPRF are acknowledged for phosphatase by which insulin resistance and type 2 diabetes is deteriorated. JS-003 is sorted as a strong inhibitor of these phosphatases according to our lab database containing inhibition ability of 658 natural compounds in human-derived phosphatases. We conducted on research to determine IC50 value which represents inhibition ability of JS-003 in phosphatases followed by experiments to probe the efficacy of JS-003 for improving glucose-uptake ability in mammalian cells. Our results of experiments show that JS-003 is a potential therapeutic compound for type 2 diabetes.

Poster Presentation : **LIFE.P-303**
Life Chemistry
Zoom 7 WED 17:30~18:00

Identification of a natural product inhibitor for Src-homology phosphotyrosyl phosphatase 2

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cardiovascular disease, neuropathy, kidney damage, and so on. There are two types of diabetes: type 1 diabetes (T1D) and type 2 diabetes (T2D). Especially type 2 diabetes (T2D) is occurred by a disability of glucose uptake and is mainly related to insulin resistance. Src-homology phosphotyrosyl phosphatase 2 (shp2) is one of the targets for type 2 diabetes (T2D). It has been reported that overexpression of SHP2 causes various types of cancer: obesity and diabetes. Therefore, the Inhibition of SHP2 activity can improve type 2 diabetes (T2D) by enhancing insulin sensitivity. In order to identify a potential therapeutic compound for diabetes, 658 natural compounds were screened by enzyme kinetics and selected by C2C12 cell viability test. SHP2 expression and purification proceeded for enzyme kinetics and IC50 and Ki were examined. Also, we confirmed whether SHP2 is a target for diabetes by performing siRNA knockdown. These results implicate that JK102 could be a therapeutic target for diabetes.

Poster Presentation : **LIFE.P-304**
Life Chemistry
Zoom 7 WED 17:30~18:00

Antidiabetic effect of MJ44 polymeric micelles targeting protein tyrosine phosphatases

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Micelles are nanoparticles as be used for targeted drug delivery. Targeting drug delivery systems such as liposomes and polymeric micelles make numerous chemotherapeutics available that are too toxic to use. Drug-loaded micelles enhance water solubility and circulation time of drugs. Furthermore, they can target specific tissues via enhancing retention effect. To improve the antidiabetic effect using these effects, we have made micelle using MJ44, MJ84, and MJ28. MJ84 is an amphipathic compound, thus it performs the packing behavior. MJ28 is an antidiabetic substance selected according to bioinformatics and helps to form micelles. Also, it indicated experimentally protein tyrosine phosphatases (PTPs) inhibitor. MJ44 inhibited diabetes-related PTPs such as SHP2, PTP-MEG2, DUSP9, TC-PTP, PTP-sigma in vitro. MJ44 micelles, MJ44, MJ84, and MJ28 did not exhibit cytotoxicity in C2C12 cells. These results suggest MJ44 polymeric micelles are a potential therapeutic candidate for diabetes.

Poster Presentation : **LIFE.P-305**
Life Chemistry
Zoom 7 WED 17:30~18:00

Target analysis of herbal medicine prescription related to diabetes by high-throughput screening and network analysis

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Traditional oriental medicine (TOM) has been used to treat disease for thousands of years. However, the targets of TOM have been barely validated by modern analytical science because TOM has been established by qualitative and philosophical approach. To create the method which reveal the target of TOM ingredients by analytical science, we have accumulated a set of biological data based on in vitro enzyme assay with high-throughput screening (HTS) of 658 purified natural products for inhibition of human protein tyrosine phosphatase (hPTP) libraries consisting of 77 members. The resulting data were combined with the data of herbal medicine, which affords pre ready data for systemic analysis of disease, medicinal target, natural product, herbal medicine, prescription of herbal medicine for type 2 diabetes (T2D). Ingredients included in the diabetes-related herbal medicine prescription have been shown to inhibit diabetes-related PTPs. Among herbal medicine prescriptions for T2D, 14 showed targeting of T2D related PTPs and the most targeted PTP was PTPN11. This is the first example that a set of prescriptions for a specific disease was validated by modern analytical science. The result supported that TOM has each medicinal target for specific disease. This type of analysis may pave a way to validate TOM and to discover novel medicinal targets at the same time.

Poster Presentation : **LIFE.P-306**
Life Chemistry
Zoom 7 WED 17:30~18:00

Enhanced Biocompatibility of 3D cartilage scaffolds with decellularized ECM based hydrogels

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Bio-printing hydrogel is a technique that is used in broad areas of tissue engineering. Hydrogel must have good biocompatibility, cytocompatibility, biodegradability, printability, and mechanical properties to apply scaffold for tissue engineering. Biomaterials like alginate, agarose, gelatin, hyaluronic acid, and collagen are mainly added to hydrogel. Variety of methods, for example, keeping good hydrophilicity for good cell encapsulation, mimicking the natural microenvironment of the tissue to increase biodegradability, adjusting viscosity to self-retain the structure after 3d-printing, adding extracellular matrix on hydrogel, and modulating the pore size for cell attachment are used to make hydrogel have appropriate properties. In this study, decellularized extracellular matrix (d-ECM) is added to increase cell viability in scaffold. d-ECM has big advantage that it has many components such as cell adhesive proteins, growth factors, collagen, proteoglycan, fibronectin and laminins that help cells grow in bio-printed scaffold. Also because d-ECM is decellularized form of ECM, potential antigens are removed that it causes much lower immune and inflammatory responses after implantation in vivo. Using this advantages of d-ECM, diverse scaffold can be made that are applicable to human body. We are studying on basic physical properties, mechanical properties, and biocompatibility of this d-ECM added hydrogel with GelMA, alginate and PEGDA.

Poster Presentation : **LIFE.P-307**

Life Chemistry

Zoom 7 WED 17:30~18:00

Napthalimide appended deoxyuridine nucleotide synthesis and application in detection of miRNA 24-3P through Rolling Circle Amplification

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In here, we synthesized a highly fluorescent Naphthalimide impeded deoxy uridine triphosphate, by taking advantage of its aggregation-induced emission property we successfully incorporated and applied this triphosphate for detection of miRNA 24-3P through rolling circle amplification. Up on rolling circle amplification the multiple dUrkTP substituted DNA with large than 10 kb will form a gel which induce aggregation to enhance the fluorescence signal. This probing system is simple direct incorporation and extension into rolling circle product provide an opportunity to detect the miRNAs (limit of detection: 3.37 fM) which are found in very low concentration.

Poster Presentation : **LIFE.P-308**

Life Chemistry

Zoom 7 WED 17:30~18:00

Enzymatic primer extension of unnatural nucleotide into DNA and its combination with Graphene Oxide for detection of miRNA21

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Herein we designed new diagnostic method to detect miRNA21 via enzymatic primer extension of unnatural nucleotide with Morpholine naphthalimide deoxyuridine(dUrkTP) which is our research group have been developed. We tried to incorporate dUrkTP into DNA using DNA polymerase and separated dUrkTP including primer(rkDNA) using Lambda exonuclease and combined with Graphene Oxide(GO) for the detection of miRNA 21. rkDNA exhibited strong fluorescence but fluorescence was quenched in the presence of GO. This rkDNA-GO system showed enough selectivity and sensitivity for the detection of miRNA21 and it also exhibited short detection time that is around 30minutes. We believe that other types of miRNA also would be detectable by this probing system.

Poster Presentation : **LIFE.P-309**

Life Chemistry

Zoom 7 WED 17:30~18:00

Biophysical properties of Infliximab

Soon-Jong Kim[*], Eun Hye Park[1]

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Infliximab is a monoclonal antibody works against tumor necrosis factor alpha (TNF-a) for treatment of autoimmune diseases including rheumatoid arthritis and Crohn’s diseases. Original patent of the antibody belongs to Janssen Biotech (Remicade). Biosimilars of the Remicade are commercially available (such as Remsima, Celltrion). In this work, we present the stability and oligomeric natures of Remsima by using fluorescence and analytical ultracentrifugation (AUC) techniques.

Poster Presentation : **LIFE.P-310**

Life Chemistry

Zoom 7 WED 17:30~18:00

Unveiling Terminal Residue-Dependent Electrostatic Interactions in Circularly Permuted and Split Outer Membrane Protein

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Outer membrane protein (Omp) has a critical role in small molecule and protein translocation, as well as signal transduction. The Omp folding into the outer membrane of gram-negative bacteria have been well known to be assisted by β-barrel assembly machinery complex. However, the chemical mechanisms of spontaneous folding into outer membrane have not yet been elucidated. Here, we carried out circular permutation, split and complementation, and point mutation of outer-membrane protein F (OmpF), one of the most abundant and functional β-barrel proteins in gram-negative bacteria. By altering the terminal residues, which expected to interact with lipid head group during folding into membrane, we demonstrate that the terminal residues affect the folding efficiency and kinetics of circularly permuted OmpF. Our results suggest that the folding of the native β-barrel integral membrane proteins is tightly controlled, downregulating non-enzymatic and spontaneous folding process. In addition, our work provides unprecedented strategy for improving folding efficiency of β-barrel membrane protein in various applications.

Poster Presentation : **ORGN.P-311**
Organic Chemistry
Zoom 6 WED 16:30~17:00

New Blue Phosphorescent Heteroleptic Ir(III) Complexes with Imidazole- and *N*-Methylimidazole Carboxylates as Ancillary Ligands

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Department of Chemistry, Pusan National University, Korea

Imidazole- and *N*-methylimidazole carboxylate have been introduced to serve as ancillary ligands in heteroleptic Ir(III) complexes containing 2-phenylpyridine-based main ligands, with consideration of the frontier orbital energy levels. Complexes **Ir1**−**Ir4** were synthesized and found to have LUMO levels higher than that of the corresponding Ir(III) complex containing pyridyl carboxylate. All the synthesized Ir(III) complexes exhibited blue phosphorescence emission maxima in the region of 465−467 nm at room temperature. Phosphorescent quantum efficiencies were increased by a factor of 1.8−6.7 by blocking the intermolecular hydrogen bonding between the imidazole carboxylate ligands of neighboring Ir(III) complexes, which was achieved by *N*-methylation of the imidazole carboxylate ancillary ligand. The organic light-emitting diodes fabricated using **Ir3** and **Ir4** as dopant materials in the emissive layers were found to emit blue emission with peaks at 469 and 471 nm and maximum external quantum efficiencies of 20.0 and 22.4%, respectively. Moreover, all the fabricated devices with **Ir3** and **Ir4** exhibited low efficiency roll-off, indicating excellent stability of the materials.

Poster Presentation : **ORGN.P-312**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Thienyl group effect of BDT based on Fluorinated Phenazine

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[1]*Department of Polymer Engineering, Pukyong National University, Korea*

Solar cells are in the spotlight as one of the eco-friendly energy. But efficiency is still a problem for solar cells to be commercialized, so we used a D-A structure which can controls energy levels of polymers to formulate proper energy level of polymers. Difluorinated phenazine(DFPz) composed of butyl octyl alkyl chain was used as an accepter unit, and difference of performance was compared by using BDT and BDTT as a donor unit. As a result, polymer with BDTT showed better performance than polymer with BDT. The HOMO of BDTT-DFPz was reported lower than that of HOMO of BDT-DFPz, which resulted in increased Voc. FF were also improved, giving BDTT-DFPz better PCE. This was predicted to have expanded π conjugated structure due to the added thiophene, which may have improved the charge mobility. Therefore, it was found that BDTT-DFPz showed 5.28% PCE, whereas BDT-DFPz showed 4.24% PCE.

Poster Presentation : **ORGN.P-313**

Organic Chemistry

Zoom 6 WED 16:30~17:00

DABCO-Mediated Synthesis of α-Trifluoromethylthio-α,β-Unsaturated Carbonyl Compounds

Heun-Jong Ha, Junho Park, Chang-Woo Cho*

Department of Chemistry, Kyungpook National University, Korea

The introduction of the trifluoromethylthio group (–SCF_3) into bioactive molecules often results in significant improvement in cell membrane permeability, which in turn enhances bioavailability. Therefore, the –SCF_3 group has recently attracted considerable attention, and intensive efforts have been devoted to develop efficient synthetic routes to incorporate the –SCF_3 group into organic compounds. Furthermore, electrophilic α-trifluoromethylthiolations of carbonyl compounds have been actively researched in order to synthesize α-SCF_3-carbonyl compounds. However, electrophilic α-trifluoromethylthiolations of α,β-unsaturated carbonyl compounds have been much less explored despite the importance of α-SCF_3-α,β-unsaturated carbonyl compounds as building blocks for pharmaceuticals and agrochemicals. Herein, we report a DABCO-mediated direct α-trifluoromethylthiolation of α,β-unsaturated carbonyl compounds without β-substituents using an electrophilic SCF_3 source that affords the corresponding α-SCF_3-α,β-unsaturated carbonyl compounds in good yields.

Poster Presentation : **ORGN.P-314**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Synthesis and chiral analysis of various gamma modified PNA backbones

Alagarsamy Periyalagan, **In seok Hong**[1,*]

Department of chemistry, Kongju National University, Korea

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Peptide nucleic acid is a DNA/RNA analog, in which the sugar-phosphate backbone has been replaced by a unit of N-(2-aminoethyl) glycine. PNAs are used as an emerging diagnostic tool or therapeutic agents in day to life. Due to aggregation and the lack of water-solubility properties of PNAs, so many modifications have been done at monomeric level. Introduction of chiral center at α, β, γ position of the backbone in PNA can overcome these difficulties. In the case of inserting a chiral center at the γ position chance to produce enantiomeric impurities, it is unacceptable in biologically active molecules. Here, we have prepared various gamma modified PNA backbones such as lysine, glutamate, histidine, alanine, arginine, and serine moieties using different synthetic strategies. Chiral purity of each backbone was measured by introducing of Fmoc-leucine and Fmoc-alanine to the secondary amine of each backbone. The overall results from HPLC analysis showed that the Red-Al used pathway at -20°C condition offered as much as chiral pure products in reasonable yields.

Poster Presentation : **ORGN.P-315**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Synthesis and characterization of Aurein 1.2 peptides using solution phase synthesis

Jiseon Kim, Yonghoe Kim, In seok Hong[1,*]

Chemistry, Kongju National University, Korea

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

Aurein 1.2 peptide is a membrane-permeable peptide found in a frog (Litoria aurea). As part of a drug delivery system, many studies have been conducted to effectively deliver drugs to target cells by combining aurein 1.2 with drugs. In general, short peptides can be easily synthesized through solid phase peptide synthesis, but for mass production, it is efficient to synthesize peptides by solution phase synthesis. Here, we successfully synthesized aurein 1.2 on the scale of several tens of grams by the solution-phase peptide synthesis. For efficient synthesis, the peptide was divided into several blocks, and the final aurein 1.2 was assembled by sequentially coupling the blocks. Various coupling reagents were tested to minimize epimerization in each block-coupling step, and optimal synthetic conditions were applied. A fully protected Aurein 1.2 peptide was synthesized, purity was identified by HPLC, and mass was identified by MALDI-Tof. In the future, we plan to study the cell delivery efficiency by conjugating the synthesized aurein 1.2 peptide with various drug candidates.

Poster Presentation : **ORGN.P-316**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Optimization of peptide coupling agents to minimize racemization in the synthesis of poly Histidine peptide in solution phase

Ji in Kim, In seok Hong*

Department of Chemistry, Kongju National University, Korea

Poly-histidine is known to facilitate endosome escape in poly-histdidine conjugated drugs. In addition, as it is used as a cell penetrating peptide (CPP), it can deliver pharmacological substances such as DNA or proteins that cannot pass through the cell membrane without damaging the cell membrane. Solid-phase peptide synthesis, which is generally used in peptide synthesis, has several disadvantage in that it uses an excessive amount of agents and is difficult to synthesize on a large scale. In this study, fully protected poly-histidine was synthesized by solution-phase peptide synthesis, which is easy to apply for large-scale synthesis. There are many reports in the literature that racemization occurs during coupling between peptide blocks. In this study, coupling reagents that minimize racemization during block coupling were investigated under various conditions. A fully protected poly-histidine (Fmoc-His(Trt)$_{10}$-O-OMe) was successfully synthesized using an optimized coupling reagent.

Poster Presentation : **ORGN.P-317**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Derivatization of Peptoid Using Petasis Borono-Mannich Reaction

Minhwa Kim, Yong-Uk Kwon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Along the drug development history, there are increasing needs for the development of new chemical tools possessing improved bioactivities, pharmacokinetics, etc. Peptoids, a series of N-substituted oligoglycines, are one of the fascinating peptidomimetics which have many advantages over peptides. In peptoid chemistry, many ligation strategies for structural diversity have been developed to produce interesting peptoid derivatives and some of them have been also employed as macrocyclization methods to afford cyclic peptoids or more complex peptoid structures. In addition to our efforts in these studies, Petasis borono-Mannich reaction (PMR) which is one of multicomponent reactions was investigated for peptoid derivatization. Petasis borono-Mannich reaction is a multicomponent reaction in which three components of an amine, a carbonyl compound, and a aryl boronic acid participate to form substituted amines under mild reaction conditions which should be advantageous in solid-phase reactions. In this study, we envisioned three different approaches employing amine-anchored, boronic acid-anchored, and acetal-anchored peptoids on beads. The conversion efficiency was promising when amine-anchored and boronic acid-anchored peptoids were treated with other necessary components on solid phase. However, acetal-anchored peptoids as carbonyl precursors did not work well. On the other hand, PMR-based macrocyclization was also attempted to afford cyclic peptoids even though further investigation is needed.

126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **ORGN.P-318**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Construction of Complex Peptoid-Based Structures

Soomin Kim, Yong-Uk Kwon*

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Peptoids, N-alkylated glycine oligomers, have emerged as an attractive class of peptidomimetics which possess many characteristic advantages over peptides, including easy synthesis of libraries, proteolytic resistance and improved cell permeability. In addition, structurally rigid cyclic peptoids have been in the spotlight for their improved cell permeability, higher proteolytic resistance, and stronger binding affinity against target proteins. Moreover, more complex peptoid structures should be assumed to contain interesting structural features and promising potentials as molecular probes, molecular transporters, or chemical tools in the field of chemical biology and molecular recognition. Development of the synthetic strategies is also very challenging.For the development of novel peptoid-based structures, we have envisioned to construct bridged peptoids, sandwich-type peptoids, sphere-type peptoids, etc. We could get the high conversion efficiency in the construction of bridged peptoids and sandwich-type peptoids. Additionally, we have designed and synthesized sphere-type peptoids through the combination of chemically orthogonal macrocyclization strategies such as macrolactamization, disulfide-bond formation and ring-closing metathesis. In this presentation, we will introduce our efforts on the development of complex peptoid-based structures in three dimension.

Poster Presentation : **ORGN.P-319**
Organic Chemistry
Zoom 6 WED 16:30~17:00

The Study on New Alternating Polymers Having BDTT and Phenazine for Photovoltaics

Jinhan Lee, Won Ki Lee[1], Youngeup Jin*

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[1]*Department of Polymer Engineering, Pukyong National University, Korea*

Now days, Global energy issues are getting attention. Solar cells are being studied to solve the energy problem. Solar cells in D-A structure have been studies. These polymers were consisted of Benzodithionylthiophene that electron-donor unit and phenazine that electron-acceptor unit. Three type of Phenazine derivatives were choosed. One is Dodecyl alkyl chain that is linear and the other is two 2-Butyl octyl, 2-decyl hexyl alkyl chain that is bulky. Comparing with linear alkyl chain and bulky alkyl chain, the later is better performance than the former. Because Phenazine's bad solubility. Linear alkyl chain caused the problem of cohesion. So it cause low PCE of 2.73%. And then comparing with two bulky alkyl chain, 2-butyl octyl and 2-decyl hexyl, the former chain has better performance than the later. Because former polymer have good crystallization properties. The later is too bulky so its crystallization properties low degree and it cause low PCE of 2.76%. But 2-butyl-octyl phenazine has proper size. So it can draw out high performance of PCE of 5.28%

Poster Presentation : **ORGN.P-320**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Enhanced Thermoelectric Performance of SWNT/Organic Small Molecules (OSMs) Hybrid Materials by Tuning the Energy Level of OSMs

Jong-in Hong[*], **Tae-hoon Kim**[1]

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

Global shortages of the fossil fuel trigger the needs of alternative renewable energy conversion techniques. In this context, thermoelectric (TE) materials are potent candidates for renewable energy generation as TE materials immediately recover disused heat to utilizable electrical power by harnessing a temperature gradient. TE performance is generally estimated by dimensionless figure of merit, ZT ($ZT= S^2\sigma T /\kappa$), which consists of the Seebeck coefficient (S), the electrical conductivity (σ), thermal conductivity (κ), absolute temperature (T), and power factor (PF, $S^2\sigma$). To fabricate high-performance TE generator, S, σ, and κ values should be meticulously controlled. However, these three parameters are intercorrelated, hampering the rapid development of highly efficient TE devices applicable in real life. In this regard, tailored single-walled carbon nanotube/organic small molecule (SWNT/OSM) hybrid materials have drawn significant attention as they possess high S and low κ originated from OSMs as well as excellent conductivity from SWNT. Until now, systematically tuning the electronic level of OSMs was not utilized for the simultaneous increment of the S and PF.

Herein, we synthesized four π-conjugated OSMs, **dCNBT**, **PBT** (as a control), **mBT**, and **dmBT**. The energy levels of the four OSMs were adjusted by introducing electron-donating or electron-withdrawing groups onto the π-conjugated backbone. Our study revealed that both S and PF can be improved by fine-tuning of the HOMO levels and Eg values of OSMs. This is an excellent example of enhancing thermoelectric performance by controlling the energy level of OSMs.

Poster Presentation : **ORGN.P-321**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Stereochemical Revision and Total Synthesis of Biemamides B and D

Hyun-Joon Ha*, Nikhil Srivastava[1]

Department of Chemistry, Hankuk University of Foreign Studies, Korea

[1]*Hankuk University of Foreign Studies, India*

Anefficientlinearsyntheticroutehasbeendevelopedforthefirsttotalsynthesisof5,6-dihydrouracilcontainingmarinenaturalproductsbiemamidesBandDaspotentialTGF-βinhibitorsfromcommerciallyavailableenantio-pureaziridine-2-carboxylate.Thissyntheticstrategycanbeusefulforthetotalsynthesisofotherbiemamides(A,CandE)marinenaturalproducts.Keyfeaturesofourtotalsynthesisincludesregio-andstereoselectiveaziridineringopeningviaazide,base-inducedcyclizationandsequentialpeptidecouplingreactions.AftermeasuringtheopticalpropertiesandECDspectraofbothenantiomers,theabsoluteconfigurationofnaturalbiemamidesBandDhasbeenrevisedas(–)-(5S).Itisanenantiomeroftheoriginallyproposedstructure(–)-(5R).

Poster Presentation : **ORGN.P-322**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Optical and Physical Properties Correlation of π-conjugated Pyrazine Derivatives According to Different Conjugation Type.

Young Dae Gong*, Hyungha Park

Department of Chemistry, Dongguk University, Korea

In this report, various π-conjugated pyrazine derivatives were compared in many ways to study their correlation. Nonlinear optical properties such as hyperpolarizability were studied through density functional theory (DFT) calculation. Compounds were synthesized via Suzuki and Sonogashira coupling reaction using microwave irradiation and characterized using UV-vis absorption and photoluminescence to observe the optical properties. The tendency of the optical property depended on where and how many phenyl rings and triple bonds were. In general, it was found that materials with longer conjugation had a large stoke shift. Besides, a wide range of solvatochromism, acidochromism, aggregation-induced emission (AIE), and aggregation-caused quenching (ACQ) were observed. These features can later be used for chemosensors, which later has high potential value. Finally, thermal features were measured with differences scanning calorimetry (DSC) and thermogravimetric analysis (TGA), and the bulky material showed generally higher thermal stability.

Poster Presentation : **ORGN.P-323**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Synthesis of Idebenone derivatives and confirm of bioactivity with cell

Songmi Bae, Dai Il Jung*, Ju Hyun Song*

Department of Chemistry, Dong-A University, Korea

Idebenone is a drug that was initially developed by Takeda Pharmaceutical Company for the treatment of Alzheimer's disease and other cognitive defects. An important prerequisite for the success of any drug for this disease is that of crossing the blood brain barrier (BBB) even though this barrier is disrupted at the brain-tumour interface. One such compound that has been shown to cross the BBB following is idebenone. Chemically, Idebenone is structurally similar to the naturally occurring Coenzyme Q10, in that both possess a benzoquinone moiety involved in electron transport, but their hydrophobic tails differ in length and composition. The shorter tail of Idebenone seems to be the ideal length for favouring partitioning into the mitochondrial membrane and for a better BBB permeation compared to Coenzyme Q10. Recent research suggests that Idebenone may also have potential use as an anti-cancer agent. studied the effect of Idebenone on human dopaminergic neuroblastoma SHSY-5Y cells demonstrating that the mechanism of cell death was apoptotic in nature. showed that in prostate cancer cells and in pancreatic ductal adenocarcinoma cells, Idebenone reduced cell proliferation, inhibited cell migration and induced apoptosis by inhibiting anoctamin 1. This experimental purpose is developing of new anti cancer drug. Strategic design is change ester from alcohol that Idebenone functional group with esterification. We selected idebenone by bioactive alcohol with various acid. First, we synthesized of idebenone with straight chain acid, Second, we synthesized with branched chain acid and NSAIDs. We expect high effect of anti cancer of Idebenone derivation. Third, We comfirmed of bioactivity with various anti cancer cell. Next step, we plan to study bioactivity within animals.

Poster Presentation : **ORGN.P-324**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Dearomative synthesis of cyclic N-acyl amidine from N-heteroarenes and acylazide

Dong Geun Jo, **Seewon Joung**[1,*]

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

We report a synthesis of cyclic N-acyl amidine by utilizing [3+2] cycloaddition of acyl azide and enamine intermediate synthesized from the borane catalyzed dearomatization of N-heteroarenes. In the previous investigation, it was reported that acyl azide is less reactive than sulfonyl azide, so that the reaction of enamine intermediate and acyl azide cannot proceed. During the investigation of the reactivity of azide, we found that the EWG on the azide stimulate the reactivity of azide. Utilization of the EWG functional groups to azide was the key to achieve the cyclic N-acyl amidine product.

Poster Presentation : **ORGN.P-325**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Electrochemical Synthesis of Sulfone Derivatives

Jin Kyu Park[*], **Sunwoo Lee**[1]

Department of chemistry, Chonnam National University, Korea
[1]*Department of Chemistry, Chonnam National University, Korea*

Electrosynthetic methods have only recently gained significant attention, even though the concept had already been introduced over 100 years ago. There are many advantages to employing electrochemistry in organic synthesis. It provides mild reaction conditions and is environmentally friendly. The mechanism of anodic oxidative coupling reactions may be very similar to that of photo-oxidative coupling reactions because they all involve redox chemistry. We paid attention to the synthesis of vinyl sulfones by using electrochemical reaction. Herein, we present the oxidative reaction of aryl sulfonylhydrazides with aliphatic amines to provide the corresponding vinyl sulfones in good yields.

Poster Presentation : **ORGN.P-326**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Synthesis of Tetrazole *N*-Oxide Derivatives

Heun-Jong Ha, **Chang-Woo Cho**[*]

Department of Chemistry, Kyungpook National University, Korea

Terazoles are an important class of energetic materials due to their intrinsic energetic characteristics resulting from heats of formation and high nitrogen contents. Recently, considerable efforts have been put into the synthesis of tetrazol *N*-oxides as high-energy density materials for civilian and military purposes owing to their excellent performance, stabilities and low sensitivities. Therefore, the development of an efficient route for the synthesis of diverse tetrazol *N*-oxide derivatives is highly desirable. Here, we report the efficient synthesis of tetrazol *N*-oxide derivatives.

Poster Presentation : **ORGN.P-327**

Organic Chemistry

Zoom 6 WED 16:30~17:00

Synthesis of Copper Complexes with Tridentate Tris-*N*-Heterocyclic Carbene: Application to Alkyne-Azide Cycloaddition Reaction

Yeon Joo Cheong, Hye-Young Jang[1,*]

Department of Energy System Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

N-Heterocyclic carbene (NHC) ligands provide a strategic advantage in synthesizing stable transition metal catalyst complexes. Therefore, the synthetic methods of transition metal complexes with NHC ligands were well developed. Because NHC ligands have strong sigma donation ability, metal ions can coordinate strongly, allowing the complexes to be oxygen and moisture stable. In this study, we synthesized a new type of NHC ligands and used them to synthesize new copper catalysts. The three imidazolium rings of the ligand were linked through the alkyl chain. The carbenes were coordinated to copper and the structures were identified by single crystal, XANES, and EXAFS. They were applied to the alkyne-azide cycloaddition reaction. In this presentation, the synthesis and detailed characterization of copper complexes along with the catalytic results of cycloaddition will be discussed.

Poster Presentation : **ORGN.P-328**

Organic Chemistry

Zoom 6 WED 16:30~17:00

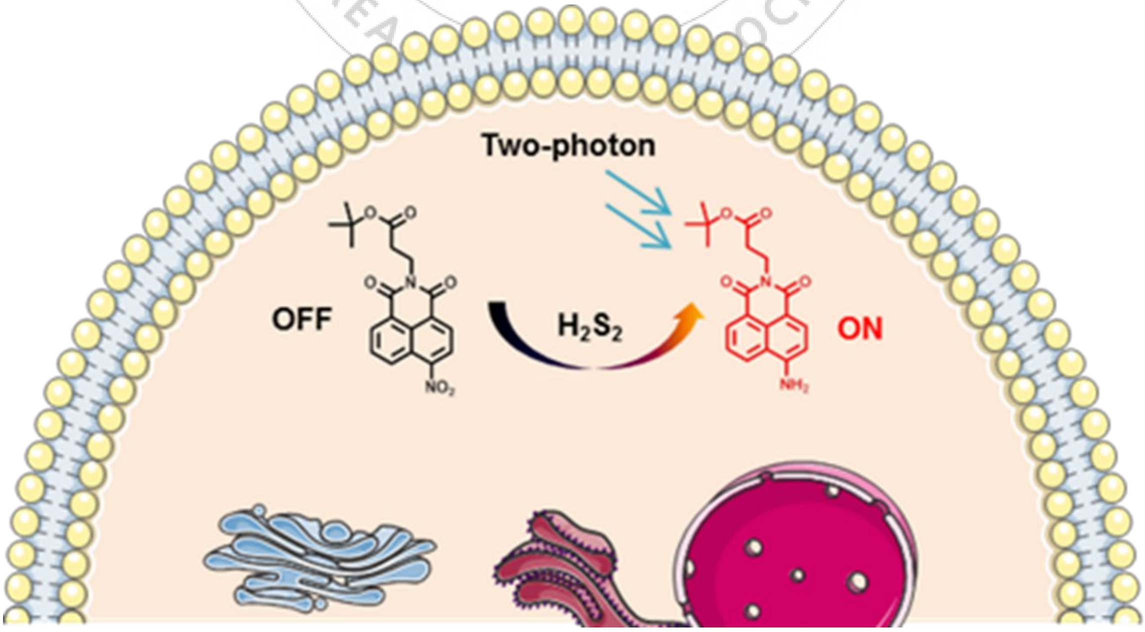
Hydrogen Polysulfides (H_2S_2) Imaging in Live Cells and Hippocampal Tissues Using Two-photon Confocal Imaging

Jeewon Chung, Hwan Myung Kim[1,*], Juyoung Yoon[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

[1]*Department of Energy Systems Research, Ajou University, Korea*

Hydrogen polysulfide (H_2S_n) plays a significant role in the pathological and physiological activities of an organism, thus it's becoming an emerging topic of research. Therefore, it may be useful to visualize the H_2S_n activity in living cells. In this work, a fluorescent probe named NI-H_2S_2 was developed as a molecular tool for detecting hydrogen polysulfides in solutions and live HeLa cells, which is based on a naphthalimide skeleton. With a two-photon fluorescence microscope, hydrogen polysulfides in hippocampal tissue of mice could also be tracked. Therefore, this probe NI-H_2S_2 is expected to serve as a practical tool for studying the physiological roles of hydrogen polysulfides in living cells and in vivo.



Poster Presentation : **ORGN.P-329**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Ir(triscarbene)-Catalyzed Transfer Hydrogenation of Levulinic Acid with Various Alcohol as a Hydrogen Source

Kihyuk Sung, Mi-hyun Lee[1], Hye-Young Jang[2,*]

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[1]*Department of Energy System Research, Ajou University, Korea*
[2]*Department of Chemistry, Ajou University, Korea*

Gamma-valerolactone is regarded as a renewable biofuel and green solvent. Various transition-metal complexes were reported for the hydrogenation of levulinic acid to gamma-valerolactone. On the other hand, transition-metal catalyzed transfer hydrogenation of levulinic acid are reported few. While the formic acid was used at most transfer hydrogenation to generate gamma-valerolactone, we utilize various alcohols as a clean and safe hydride source. In this study, we report Ir(triscarbene)-catalyzed transfer hydrogenation of levulinic acid to gamma-valerolactone using various alcohols, showing the excellent turnover number (TON) and turnover frequency (TOF).

Poster Presentation : **ORGN.P-330**
Organic Chemistry
Zoom 6 WED 16:30~17:00

Generation and Ring Opeining of N-alkylaziridinium Ions

Taehwan Yu, Hyun-Joon Ha[1,*], Won Koo Lee[2,*]

Hankuk University of Foreign Studies, Korea
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*
[2]*Department of Chemistry, Sogang University, Korea*

Non-activated aziridine bearing electron-donating substituent should be activated with electrophile with alkyl, acyl, trimethylsilyl, lewis acids, etc. prior to the ring opening reaction. Among them alkylation is quite attractive to carry both reactions on addition of alkyl group at the nitrogen and ring opening. Based on our early success to put methyl group on the ring nitrogen. We studied other alkyl groups such as ethyl and allyl substituent, all of which are ended at the nitrogen with the removal of benzyl group. In addition, we succeeded aziridine ring opeining with various nucleophiles. We would like to present the study with alkylative aziridine ring opening in regio- and stereoselective manner.

Poster Presentation : **ORGN.P-351**

Organic Chemistry

Zoom 6 WED 17:00~17:30

Palladium-catalyzed cross-coupling reaction by the use of reverse polarity of silyl ketimines

Seungmi Lee, Inji Shin*

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Ketimines are generally synthesized by the condensation with an amine and a ketone, however, the reaction is moisture sensitives and requires harsh conditions. To overcome the drawbacks, we have developed palladium-catalyzed coupling reaction to prepare various ketimines using silyl ketimines and diaryliodonium salts. The unprecedented palladium-catalyzed reactions are studied by the use of reverse-polarity of silyl ketimines. After a wide range of screening of catalysts, ligands, bases, and temperatures, we finally got the best optimized conditions for this process. A variety diaryl ketimines are effectively synthesized with tosyl-protected silyl ketimines and symmetric- as well as unsymmetric diaryiodonium salts.

Poster Presentation : **ORGN.P-352**

Organic Chemistry

Zoom 6 WED 17:00~17:30

Highly Selective Room-Temperature Suzuki-Miyaura Coupling of Bromo-2-sulfonyloxypyridines for Unsymmetrical Diarylpyridines

Young-Kyo Jeon, Wonsuk Kim[1,*]

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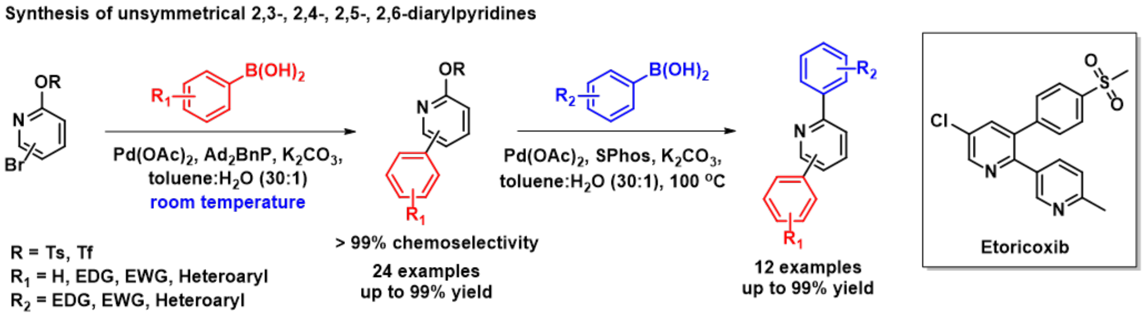
[1]*Chemistry Department of Nano-Science, Ewha Womans University, Korea*

A new and mild synthetic approach has been developed for the synthesis of pharmaceutically important unsymmetrical diarylpyridines via chemoselective Suzuki-Miyaura coupling reactions of bromo-2-sulfonyloxypyridines. Most reactions allow for facile access to aryl-2-sulfonyloxypyridines at room temperature in yields of 5-99% with excellent chemoselectivity in the presence of $Pd(OAc)_2$ (2.0 mol %) and Ad_2BnP (2.4 mol %). The second arylation of the remaining tosyl or triflyl group in the monoarylpyridine derivatives obtained was successfully accomplished for the synthesis of unsymmetrical 2,3-, 2,4-, 2,5-, and 2,6-diarylpyridine derivatives. Furthermore, a one-pot synthesis of unsymmetrical diarylpyridines starting from bromo-2- sulfonyloxypyridine was accomplished to demonstrate the practical convenience. Finally, with this method, an antibacterial agent, a topoisomerase inhibitor, and etoricoxib, a nonsteroidal anti-inflammatory drug, were successfully synthesized from the corresponding bromo-2-hydroxypyridines in overall yields of 80, 86, and 49%, respectively.



Jeon, Y.-K.; et al. *J. Org. Chem.* **2020**, *85*, 7399–7412.

Poster Presentation : **ORGN.P-353**

Organic Chemistry

Zoom 6 WED 17:00~17:30

PSCs based on D-A alternating structure with bulky alkyl chain

Jinhan Lee, Won Ki Lee[1], Youngeup Jin*

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

Recently, many studies have been conducted to increase the efficiency of PSCs. And there are many ways to increase efficiency, one of which was to use bulky alkyl chains as substituents.We wanted to create a new material for the active layer of the device. So, Diflourinated Phenazine (DFPz) and benzodithiophene(BDT) were used for alternating copolymers.Phenazine was predicted that it has good charge mobility attributed to extended π conjugated structure and it was also expected that it has strong electronegativity attributed to C=N double bonds. To investigate the effect of bulky alkyl chain, various bulkyl alkyl chain were introduced. In result, the polymer with BO(butyl octyl) alkyl chain has better performance than polymer with other bulky chain. This suggests that the BO alkyl chain is the most suitable substituent. So, the polymer with BO alkyl chain (PBDT-DT-BOFPz) achieved 4.24% of PCE (power conversion efficiency).

Poster Presentation : **ORGN.P-354**
Organic Chemistry
Zoom 6 WED 17:00~17:30

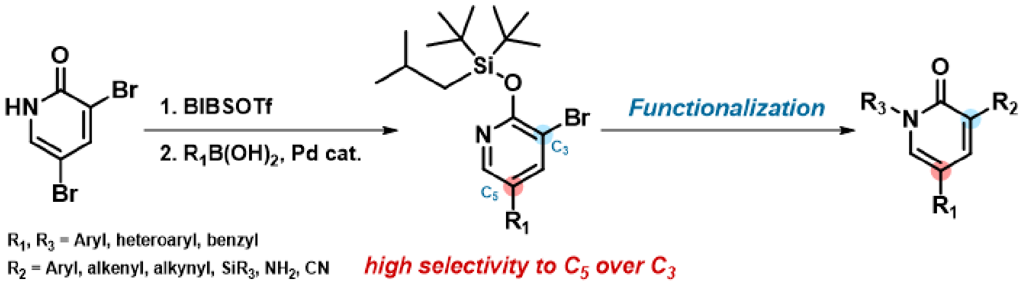
Determination of Regioselectivity using Steric-hindrance in Suzuki-Miyaura Cross Coupling Reaction

Se-Young Lim, Yong-Ju Kwon, Wonsuk Kim[1,*]

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

The regioselective Suzuki-Miyaura reaction induced by steric hindrance of 3,5-dibromo-2-silyloxypyridine was studied for the synthesis of asymmetric 3,5-disubstituted 2-pyridone. The Suzuki-Miyaura reaction proceeds well at the C5 position of 3,5-dibromo-2-(di-tert-butylisobutylsilyl)oxypyridine, with good regioselectivity. In addition, a one-pot synthesis of asymmetric 3,5-diaryl-2-pyridone starting from 3,5-dibromo-2-silyloxypyridine was carried out to prove practical convenience. Further functionalization of the remaining bromine groups, such as transition metal-catalyzed C-C, C-N and C-CN bond formation reactions and retro-brook rearrangement of C-Si bond formation to synthesize biologically relevant asymmetries 3, 5-disubstituted 2-pyridone derivatives were successfully completed. Finally, through this method, the non-glycoside cardiotonic Amrinone drug was successfully synthesized from 3,5-dibromo-2-hydroxypyridine in three steps, with a total yield of 50%.

Synthetic methods for unsymmetrical 3,5-disubstituted pyridones



R_1, R_3 = Aryl, heteroaryl, benzyl
R_2 = Aryl, alkenyl, alkynyl, SiR_3, NH_2, CN

high selectivity to C_5 over C_3

- High regioselective coupling reaction on pyridine moiety via steric effect (71-88% yield)
- Diverse bond formation reaction: ● C_3–C ● C_3–N ● C_3–CN ● C_3–Si
- Easy to eliminate the silyl protecting group for affording pyridone scaffolds (18 examples)

Poster Presentation : **ORGN.P-355**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Unexpected Formation of Diketopiperazines from Proline-based Nucleotripeptides

Chung-Min Park

Chemical Advanced Materials, Gangneung-Wonju National University, Korea

The amide bond is one of the most abundant chemical bonds and has high stability in biological systems and towards various reaction conditions. The stability of amide bonds is attributed to its nature to form the resonance structure of amide bond and it is responsible for the important biological functions. Although the amide bond is usually stable under acidic and basic reaction conditions, at high temperatures and pressure, and in the presence of other chemicals, the amide bonds in specific environments can be activated and hydrolyzed by enzymes, metal complexes, and non-metal based reactions. Besides, less reactive amide bonds presenting in biomolecules such as peptides, glycopeptides, nucleotides in oligonucleotides, and proteins can be also hydrolyzed by enzymes and metal-mediated activation. In performing our work for the development of peptide-based oligonucleotides, we observed an unexpected amide bond cleavage of tripeptides having nucleobases under mild conditions, resulted in diketopiperazine (DKP). Here, we present that the nucleobases on the triprolines increase the cis state conformations of the tripeptide skeleton, resulting in the unprecedented amide bond cleavage.

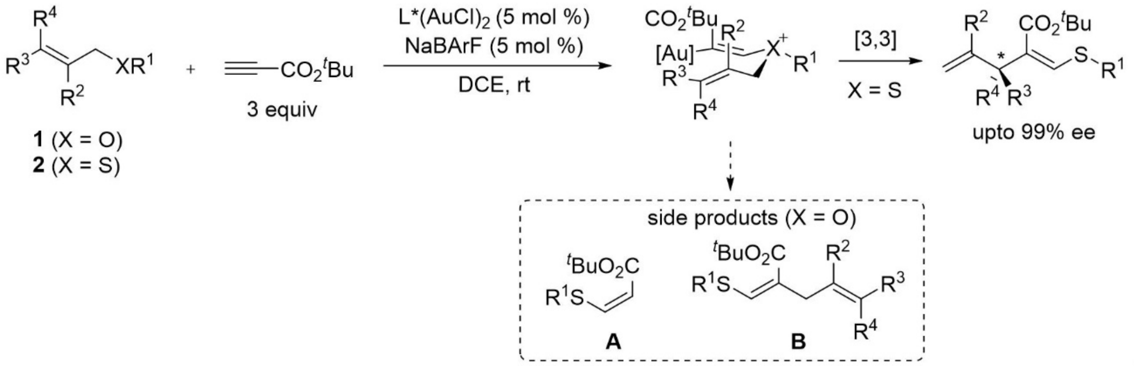
Poster Presentation : **ORGN.P-356**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Catalytic Asymmetric Thioallylation of Propiolates via Charge-Induced Thio-Claisen rearrangement.

Kim Hanbyul, Jiwon Jang, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Enantioselective intermolecular gold-catalysis is challenging, because the linear coordination geometry of Au(I) complexes imposes the approach of pronucleophiles from the opposite side of the gold. Prompted by our recent success in promoting intermolecular enantioselective coupling of propiolates and alkenes,[1] we embarked on the enantioselective alkoxylation and thioallylation of propiolates,[2] via [3,3]-sigmatropic rearrangement. The substate scope of enantioselective Claisen rearrangement has been limited to a few systems[3] and we introduced herein use of -onium intermediates for the enantioselective Claisen rearrangement for the first time. Remarkably, by replacing allyl ethers with allyl thioethers, problems such as dissociation of allyl unit (**A**) and competing [1,3]-rearrangement (**B**) could be minimized. Thus, the current Au(I)-catalyzed thioallylation allows for remarkable scope of allyl group, including highly enantioselective synthesis of all C-quaternary centers and exceptional functional group compatibility with many Lewis bases and π-groups.[4]**References**1. Kim, H.; Choi, S. Y.; Shin, S. *Angew. Chem. Int. Ed.* **2018**, *57*, 13130.2. For racemic version: (a) Jun, J.; Yeom, H. –S.; An, J. –H.; Shin, S. *Beilstein J. Org. Chem.* **2013**, *9*, 1724. (b) Park, S. R.; Kim, C.; Kim, D. –G.; Thrimurtulu, N.; Yeom, H. –S.; Jun, J.; Shin, S.; Rhee, Y. H. *Org. Lett.* **2013**, *15*, 1166.3. For experimental and theoretical studies on the substituent effects in Claisen rearrangement: (a) Curran, D. P.; Suh, Y. -G. *,J. Am. Chem. Soc.* **1984**, *106*, 5002. (b) Coates, R. M.: Rogers, B. D.; Hobbs, S. J.; Peck, D. R.; Curran, D. P. *J. Am. Chem. Soc.* **1987**, *109*, 1160. (c) O'Rourke, N. F.; Wulff, J. E. *Org. Biomol. Chem.* **2014**, *12*, 1292. (d) Geherty, M. E.; Dura, R. D.; Nelson, S. G. *J. Am. Chem. Soc.* **2010**, *132*, 11875. 4. Kim, H.; Jang, J.; Shin, S. *manuscript in preparation.*


R4
R3
XR1
R2
1 (X = O)
2 (X = S)
+
CO2tBu
3 equiv
L*(AuCl)2 (5 mol %)
NaBArF (5 mol %)
DCE, rt
CO2tBu
R2
[Au]
X+
R1
R3
R4
[3,3]
X = S
R2
CO2tBu
*
S
R1
R4
R3
upto 99% ee
side products (X = O)
tBuO2C
R1S
A
tBuO2C
R2
R1S
R3
R4
B

Poster Presentation : **ORGN.P-357**

Organic Chemistry

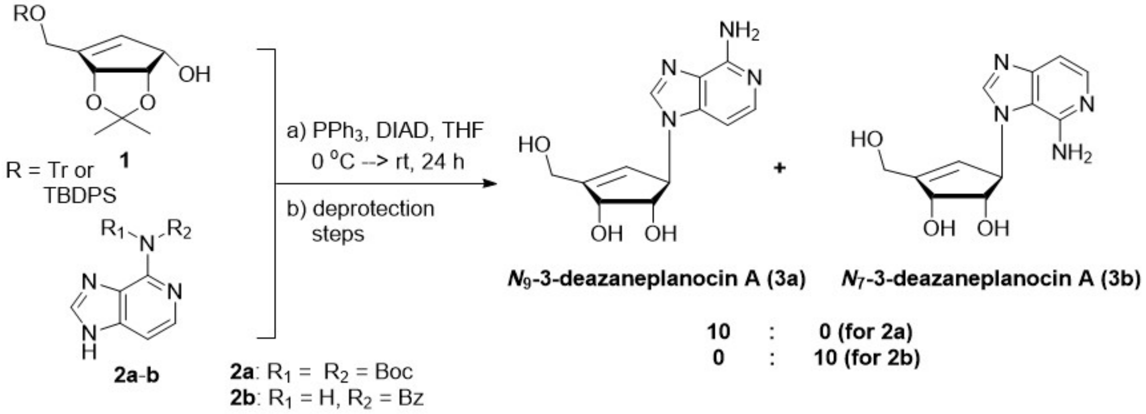
Zoom 6 WED 17:00~17:30

Regioselective Synthesis of N_7- and N_9-isomer of 3-deazaneplanocin A

SeMyeong Choi, Jin Young Lee, Yeon Jin An, Jong Hyun Cho[*]

Dong-A University, Korea

An efficiently regioselective synthesis of N_7- and N_9-3-deazaneplanocin A have been developed by using Mitsunobu reaction of N^6-protected 3-deazpurine analogs with a cyclopentenol derivative (**1**). The coupling reaction of **1** with N^6-bisBoc-3-deazapurine (**2a**) mainly provided N_9-3-deazaneplanocin A derivative in the presence of DIAD, Ph_3P in THF. Unexpectedly, the Mitsunobu reaction of **1** with N^6-Bz-3-deazapurine (**2b**) afforded only N_7-3-deazaneplanocin A in excellent yield without detection of the N_9-isomer. After removal of all protection groups, N_7- and N_9-3-deazaneplanocin A derivatives were converted into their corresponding N_7- and N_9-3-deazaneplanocin As (**3a**-**b**), respectively. In vitro assay, N_9-3-deazaneplanocin A (**3a**) showed potency against Measles (EC_{50} 0.4 μM), Flu A (H1N1) (EC_{50} 25 μM), Vaccinia (EC_{50} 2.9 μM), HCMV (EC_{50} 0.36 μM), and HBV (EC_{50} 0.59 μM). Whereas, N_7-3-deazaneplanocin A (**3b**) exhibited mild activity against Measles (EC_{50} 10 μM), Flu A (H5N1) (EC_{50} 29.0 μM), Flu B (EC_{50} 8.0 μM), HBV (EC_{50} 10 μM), and HCV (EC_{50} 22.6 μM).



Poster Presentation : **ORGN.P-358**

Organic Chemistry

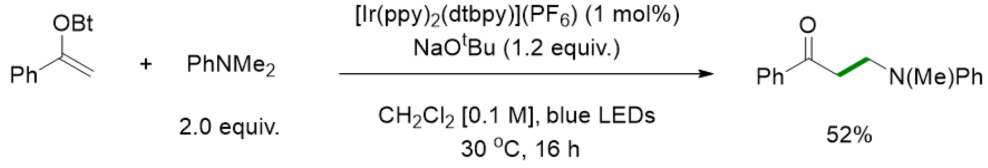
Zoom 6 WED 17:00~17:30

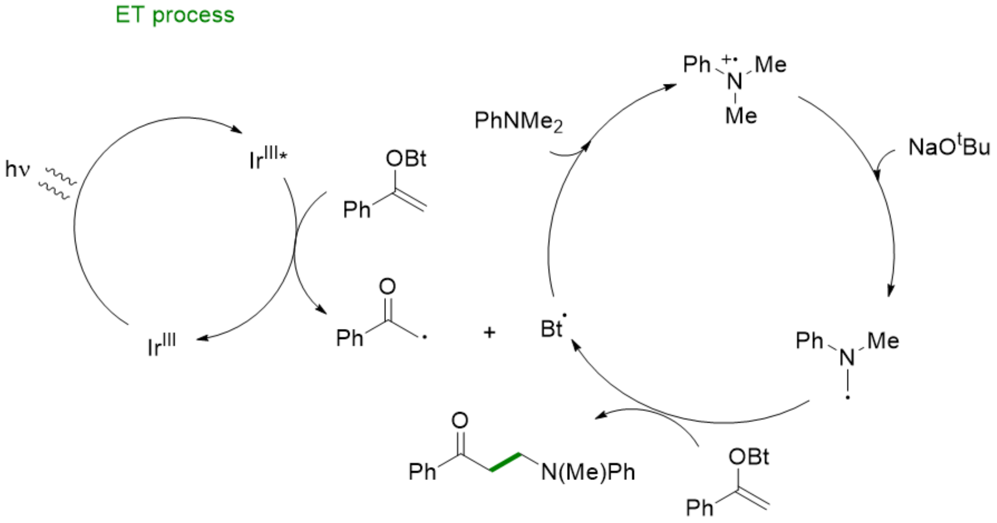
Visible Light-Enabled Radical Mannich Reaction via *sp*^{3} C-H Bond Functionalization of Tertiary Amines

Huong Quynh Nguyen, **Seunghoon Shin***

Department of Chemistry, Hanyang University, Korea

Over the past few decades, harnessing of one-electron reactivity from visible light catalysis has emerged as an appealing tool to access radical intermediates, enabling C-C and C-X bond formations.[1] In continuation of our interest in the N-O bond-mediated oxidative transformations,[2] we introduce herein enoxybenzotriazoles as substrates for the photo-catalyzed radical Mannich type reaction of tertiary amines. We envisioned that the cleavage of N-O bond by triplet state energy transfer process would produce α-carbonyl radicals and benzotriazole radicals.[3] Deprotonation of the N-centered radical cation would afford an α-amino radical which then would react with starting enoxybenzotriazole, generating β-amino ketone product, completing the radical chain.**References**[1] For recent review: Lee, K. N.; Ngai, M.-Y. *Chem. Commun.* **2017**, *53*, 13093.[2] For organometallic pathways: (a) Yeom, H.-S.; Shin, S. *Acc. Chem. Res.* **2014**, *47*, 966-977. For organocatalytic pathways: (b) Patil, D.V.; Shin, S. *Asian J. Org. Chem.* **2019**, *8*, 63-73.[3] (a) Y. Zhang, H. Liu, L. Tang, H.-J. Tang, L. Wang, C. Zhu and C. Feng, *J. Am. Chem. Soc.*, **2018**, *140*, 10695. (b) Duchemin, C.; Cramer, N. *Org. Chem. Front.* **2019**, *6*, 209-212.


OBt
Ph
+
PhNMe2
2.0 equiv.
[Ir(ppy)2(dtbpy)](PF6) (1 mol%)
NaOtBu (1.2 equiv.)
CH2Cl2 [0.1 M], blue LEDs
30 oC, 16 h
O
Ph
N(Me)Ph
52%


ET process
hν
IrIII*
IrIII
OBt
Ph
O
Ph
+
Bt
PhNMe2
Ph N Me
Me
NaOtBu
Ph N Me
O
Ph
N(Me)Ph
OBt
Ph

Poster Presentation : **ORGN.P-359**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Development of a fluorescent Probe for Diagnosis of Alzheimer's Disease

Hyeyeon Kim, Eun-Kyoung Bang[1,*]

Chemistry, Kyung Hee University, Korea
[1]Brain Science Institute, Korea Institute of Science and Technology, Korea

In the brains of patients with Alzheimer's disease, amyloid beta (Aβ) plaque and aggregated tau were observed. Recently, a correlation between aggregated tau and Alzheimer's disease has been discussed in various research reports, expecting that detecting tau aggregates may be advantageous for early diagnosis of Alzheimer's disease. Far-red fluorescent probe has a good advantage because it features non-radioactive real-time imaging, high resolution, high sensitivity, and high permeability. So, we would like to introduce a study on the far-red fluorescent tau aggregates probe that maximizes these features. We designed probes bearing the benzothiazole moiety from the known probe of tau aggregates. And we introduced the Push-Pull system for fluorescence in far-red region by introducing Dimethyl amino group as an electron donating group and nitrile group as an electron withdrawing group. We synthesized four probe candidates, and it is expected to be a selective tau binding probe through an in vitro binding assay.

Poster Presentation : **ORGN.P-360**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Synthesis and photophysical properties of methyl 2-hydroxy-4-(5-R-thiophen-2-yl)benzoate

Nam Gi Cho, Intae Kim[1,*]

Department of chemistry, Kwangwoon university, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*

Methyl salicylate derivatives have important role for surrogate of chemical warfare agents, because methyl salicylate is inert physical simulant like soman and sulfur mustard. In this study, the new methyl 2-hydroxy-4-(5-methoxythiophen-2-yl)benzoate(MHmoTB) and methyl 2-hydroxy-4-(5-cyanothiophen-2-yl)benzoate(MHncTB) were synthesized and their photophysical properties were measured in various solvents. The investigation of photophysical properties includes absorption, the luminescence and its excitation, the quantum yield, and the emission lifetime. The introduction methoxy and cyano group on 5-position of the thiophenyl of methyl 2-hydroxy-4-(thiophen-2-yl)benzoate(MHTB) causes a change in photophysical properties. The methoxy group as electron donator enhances quantum yield of deep blue luminescence in methylene chloride(MC). The cyano group as electron withdrawer produces the solvatochromism on the emission spectrum in dimethylformamide(DMF) and dimethyl sulfoxide(DMSO). Through this study, we could confirm that the introduction of the substituents (methoxy and cyano) changes the photophysical properties, so the application of various substituted derivatives is expected to be expanded.

Poster Presentation : **ORGN.P-361**

Organic Chemistry

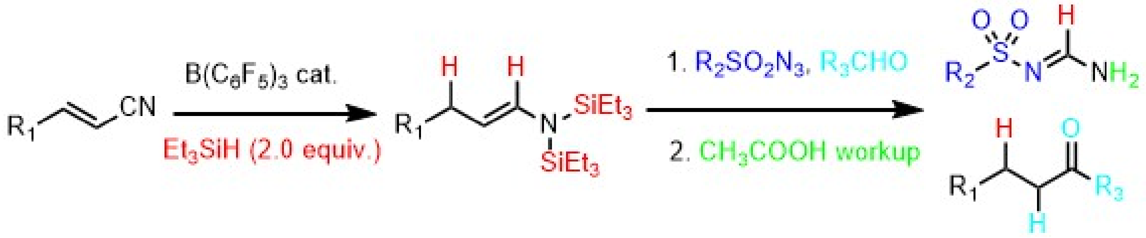
Zoom 6 WED 17:00~17:30

Cascade Borane-Catalyzed Hydrosilylation of Conjugated nitriles and [3+2] cycloaddition of organic azides: Unexpected formation of the diazoalkane and its applications

Vinh Do cao, Seewon Joung*

Department of Chemistry, Mokpo National University, Korea

We utilized borane-catalyzed partial silylative reduction of conjugated nitriles to afford N,N-disilylenamine. The intermediates from the double hydrosilylation of conjugated nitrile was subsequently react with a broad range of organic azides in situ to furnish amidines and corresponding diazo compounds via [3+2] cycloaddition and retro-[3+2] cycloaddition pathway. Diazoalkanes from retro-[3+2] cycloaddition was not stable enough for NMR observation due to the quick decomposition. To prove the retro-[3+2] cycloaddition mechanism, we tried to capture the diazoalkanes with various reagent including aldehydes which could result in development of a new cascade reaction to obtain ketone as well as amidines



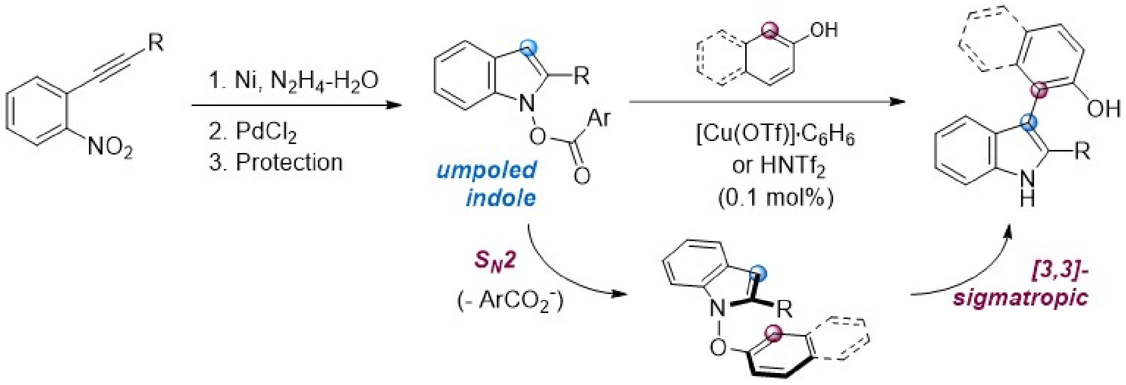
Poster Presentation : **ORGN.P-362**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Umpoled Route to Heterobiaryl Compounds via Cu(I)- or Brønsted Acid Catalysis

Soo Min Oh, Cheol Min Park[1,*], Seunghoon Shin[*]

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

Direct functionalization of inert C-H bonds is an attractive strategy and therefore have drawn intense interest. To implement such a strategy for regioselective functionalization of phenols,[1] we introduced herein *N*-benzoylindoles as electrophilic, *umpoled* indole derivatives.[2] However, direct oxidation of indoles are difficult, due to the strong aromaticity, and their synthesis have typically resorted to tedious reduction and oxidation sequences. In this presentation, we introduced our new protocol for a general synthesis of umpoled indoles, based on the electrophilic cyclization of (*o*-alkynyl)phenylhydroxylamines. Based on this, we developed two catalytic systems for *ortho*-selective coupling of phenols, namely HNTf$_2$ and [Cu(OTf)]·C_6H_6. These catalytic systems are extremely reactive and catalyze the coupling at a very low loading (0.1 mol%) and at room temperature. The unusual C2-regioselectivity was rationalized by a sequence comprising *N*-substitution, followed by [3,3]-sigmatropic rearrangement.**References**1. (a) A. P. Pulis, D. J. Procter, *Angew. Chem. Int. Ed.* **2016**, *55*, 9842. (b) Z. He, A. P. Pulis, D. J. Procter, *Angew. Chem. Int. Ed.* **2019**, *58*, 7813.2. For recent examples on synthesis of heterobiaryls: (a) H.-H. Zhan(b)g, C.-S. Wang, G.-J. Mei, Y. Li, F. Shi, *Angew. Chem. Int. Ed.* **2017**, *56*, 116. (b) S.-C. Zheng, Q. Wnag, J. Zhu, *Angew. Chem. Int. Ed.* **2019**, *58*, 1494. (c) L. -W. Qi, J.H. Mao, J. Zhang, B. Tan, *Nature Chem.* **2018**, *10*, 58. (d) C. Ma, F. Jiang, F.-T. Sheng, Y. Jiao, G.-J. Mei, F. Shi, *Angew. Chen. Int. Ed.* **2019**¸*58*, 3014. (e) C. He, M. Hou, Z. Zhi, Z. Gu, *ACS Catal.* **2017**, *7*, 5316.


R
NO_2
1. Ni, N_2H_4-H_2O
2. $PdCl_2$
3. Protection
R
N
O
Ar
O
umpoled
indole
OH
$[Cu(OTf)]\cdot C_6H_6$
or $HNTf_2$
(0.1 mol%)
OH
R
N
H
S_N2
(- $ArCO_2^-$)
N
R
O
[3,3]-
sigmatropic

Poster Presentation : **ORGN.P-363**
Organic Chemistry
Zoom 6 WED 17:00~17:30

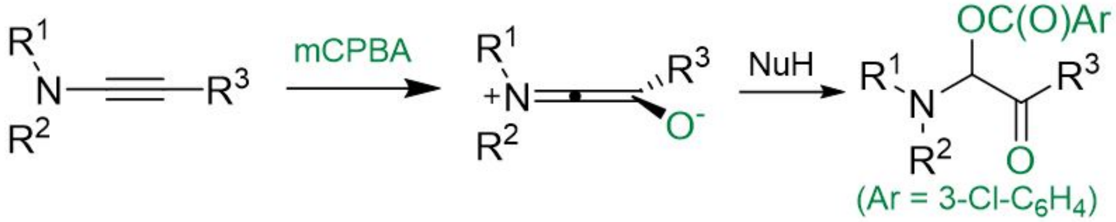
Zinc-Catalyzed Transacetalizaion of *N*,*O*-Acetals into *N*,*N*-Acetals with Benzotriazole, Indazole, and Azide

<u>SangIk Shin</u>, Seunghoon Shin[1,*]

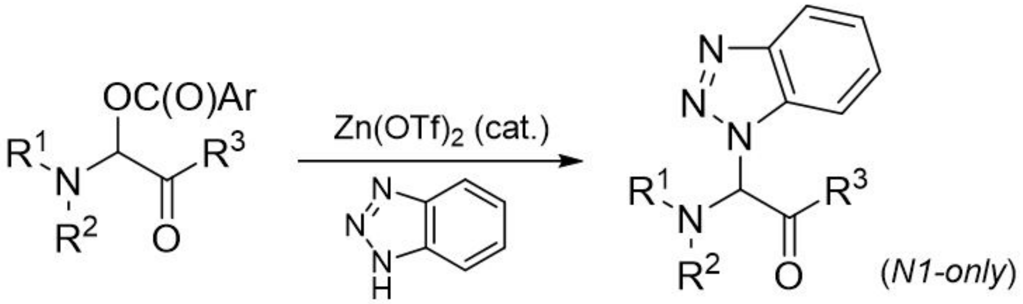
chemistry, Hanyang University, Korea
[1]*Department of Chemistry, Hanyang University, Korea*

Benzotriazoles are found as a core scaffold of a broad range of medicinal agents.[1] They can be synthesized by variety of methods, including addition to π-bonds,[2] or metal carbene,[3] alkylation through nucleophilic substitution[4] or by radical mechanism.[5] However, a mixture of N1-and N2-regioisomers are typically generated, and few of the above methods are completely regioselective.[2a,b,3] We recently reported β-oxidation ynamides prompted by *m*CPBA, β-keto-*N*,*O*-acetals.[6] In continuation of exploring the reactivity of *N*,*O*-acetals, we report herein transacetalization with bezotriazoles to form benzotriazole derivatives occurring in a highly regioselective manner.**References**1. (a) Ren, Y.; Zhang, L.; Zhou, C. -H.; Geng, R. -X. *Med. Chem.* **2014**, *4*, 640-662. (b) Suma, B. V.; Natesh, N. N.; Madhavan, V. *J. Chem. Pharm. Res.* **2011**, *3*, 375-381.2. (a) Xu, K.; Thieme, N.; Breit, B. *Angew. Chem. Int. Ed.* **2014**, *53*, 7268-7271. (b) Chen, S.-W.; Zhang, G. -C.; Lou, Q. -X.; Cui, W.; Zhang, S. -S., Hu, W. -H.; Zhao, J. -L. *ChenCatChem*, **2015**, *7*, 1935-1938. (c) Yan, W.; Ye, X.; Weise, K.; Petersen, J. L.; Shi, X. *Chem. Commun.* **2012**, *48*, 3521-3523.3. Wang, K.; Chen, P.; Ji, D.; Zhang, X.; Xu, G.; Sun, *J. Angew. Chem. Int. Ed.* **2018**, *57*, 12489-12493.4. Niedermann, K.; Früh, N.; Senn, R.; Czarnieckim B,; Verel, R.; Togni, A. *Angew. Chem. Int. Ed.* **2012**, *51,* 6511-65155. (a) Liu, Y.; Yan, W.; Chen, Y.; Petersen, J. L.; Shi, X. *Org. Lett.* **2008**, *10*, 5389–5392. 6. Nguyen, N. H.; Nguyen, Q. H.; Biswas, S.; Patil, D. V.; Shin, S. *Org. Lett.* **2019**, *21*, 9009-9013.

A. Regiodivergent oxidation of ynamides



B. Zn(II)-catalyzed transacetalization into *N,N*-Acetal (*This report*)



Poster Presentation : **ORGN.P-364**

Organic Chemistry

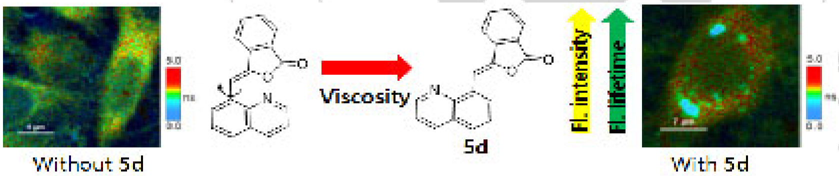
Zoom 6 WED 17:00~17:30

Systematic Modifications of a Simple Tolan: Another Category of Viscosity Sensor

Jung-Ho Hong, **Dong-gyu Cho**[*]

Department of Chemistry, Inha University, Korea

The first tolan derivative-based viscosity sensor (5d) has been synthesized, and its fluorescence intensity and lifetime increase when the viscosity of the solvent increases in methanol–glycerol mixtures. Phthalide (5d) was selected among structurally diverse tolan derivatives through systematic modifications of a simple tolan. To test 5d as a viscosity sensor, FLIM images of HeLa cells were obtained upon treatment with 5 μM of 5d for mapping the viscosity of the HeLa cells.



126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **ORGN.P-365**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Synthesis, Optimization, further Cyclization of Pyrrole Derivatives

Lina Gu, Sangho Koo[1,*]

Department of energy science technology, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Abstract Searching for an efficient transformation method of biomass into platform chemicals is an imperative and timely task for securing sustainable chemical and energy materials. A practical conversion method of monomeric carbohydrates into heterocyclic compounds was developed by the reaction with amino acid and oxalic acid in dry DMSO at 90°C based on Maillard reaction. The mild Maillard variant of carbohydrates and amino acid in heated DMSO with oxalic acid expeditiously produced the pyrrole-2-carbaldehyde skeleton. This reaction can be further improved under gradient pressure optimization conditions. Further cyclization of the highly functionalized Pyrralines afforded the pyrrole-fused poly-heterocyclic compounds as potential lead compounds for drugs ,food flavors, and functional materials.

Poster Presentation : **ORGN.P-366**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Synthesis of Norbixin and Its Ester by Bromoacetate and Julia−Kocienski Olefination Protocol

Aleksei Golikov, Sangho Koo*

Department of Chemistry, Myongji University, Korea

Norbixin 1 and norbixin ethyl ester 2 were efficiently produced with 35% and 36% overall yield respectively. Synthesis of norbixin 1 was done by coupling of ethyl bromoacetate with C20 dialdehyde 6 and following 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 demonstrated.

Poster Presentation : **ORGN.P-367**

Organic Chemistry

Zoom 6 WED 17:00~17:30

Fast Assembly and High-Throughput Screening of Structure andAntioxidant 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-368**
Organic Chemistry
Zoom 6 WED 17:00~17:30

Synthesis of Biologically Active Heterocyclic Compounds by Mn(III)-catalyzed Radical Oxidation

Miao Zhang, **Sangho Koo**[1,*]

Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Heterocyclic compounds are widely used in the pharmaceutical industry. We are trying to synthesize various heterocyclic compounds of medicinal values in an efficient way. We developed a very effective Mn/Co catalytic condition for oxidative deacetylation of the acetoacetate compounds under aerobic condition, which was utilized for the preparation of 1,4-dicarbonyl compounds. Various hetero-aromatic compounds were efficiently obtained by the Paal-Knorr syntheses from the diversely substituted 1,4-dicarbonyl compounds.

Poster Presentation : **ORGN.P-369**

Organic Chemistry

Zoom 6 WED 17:00~17:30

Synthesis of unnatural carotenoids with good electrical properties

Huijung Yang, **Sangho Koo**[1,*]

Myungji University, Korea

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

Carotenoids have a variety of beneficial effects and are particularly good at antioxidant activity. unnatural carotenoids substituted with phenyl groups have good electrical properties in addition to their advantages. Using these advantages, the electrical conductivity can be measured by replacing the terminal group with a methylthio group and attaching to the gold plat. This unnatural carotenoids can be efficiently synthesized by the julia-kocienski olefination of triene dialdehyde with BT(benzothiazole)-Sulfone. It can assemble the methylthio group through a wittig reaction with 4-thiomethylbenzyl phosphonium bromide.

Poster Presentation : **ORGN.P-370**

Organic Chemistry

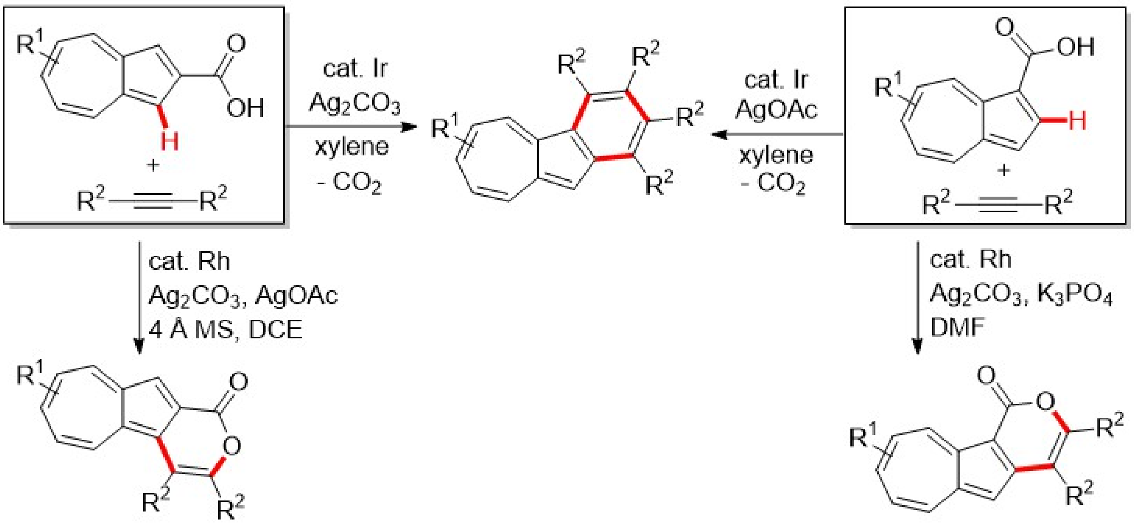
Zoom 6 WED 17:00~17:30

Expansion of Azulenes as Nonbenzenoid Aromatic Compounds for C–H Activation : Ir- and Rh-Catalyzed Oxidative Cyclization of Azulene Carboxylic Acids with Alkynes for the Synthesis of Azulenolactones and Benzoazulenes

Tae Hyeon Kim, Hee Jin Yang, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Rhodium-catalyzed oxidative [4 + 2] cyclization reactions through the C−H activation of azulene carboxylic acids as non-benzenoid aromatic compounds with symmetrical and unsymmetrical alkynes were developed under aerobic conditions, which produced azulenolactone derivatives with a wide substrate scope and excellent functional group tolerance. Interestingly, azulenic acids in the reaction with alkynes underwent an iridium-catalyzed [2 + 2 + 2] cyclization reaction accompanied by decarboxylation to afford tetra(aryl)-substituted benzoazulene derivatives. Reactivity order for C−H activation reaction is greater toward azulene-6-carboxylic acid, azulene-1-carboxylic acid, and azulene-2-carboxylic acid. For the first time, the expansion of azulenes having directing group as non-benzenoid aromatic compounds for C−H activation was successful, indicating that non-benzenoid aromatic compounds can be used as good substrates for C−H activation reaction. Therefore, research area of C−H activation will certainly expand to non-benzenoid aromatic compounds in future.


cat. Ir
Ag$_2$CO$_3$
xylene
- CO$_2$
cat. Ir
AgOAc
xylene
- CO$_2$
cat. Rh
Ag$_2$CO$_3$, AgOAc
4 Å MS, DCE
cat. Rh
Ag$_2$CO$_3$, K$_3$PO$_4$
DMF
R^1
R^2
H
OH
O

Poster Presentation : **ORGN.P-391**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Cu-catalyzed hydrocarboxylation of allenes with carbon dioxide and diisobutylaluminum hydride

SangHyun Lee, Yunmi Lee*

Department of Chemistry, Kwangwoon University, Korea

Carboxylic acids are common structural motifs of bioactive molecules and useful precursors for accessing alcohols, esters, amides, and acid chlorides. Carbon dioxide is nontoxic, inexpensive, and abundant and has been utilized as a useful C1 building block for synthesizing carboxylic acids by using organometallic reagents such as Grignard and organolithium reagents. Since these reactions are often limited to producing a variety of carboxylic acids containing functional groups, the development of new synthetic protocols that are readily available under mild conditions is highly desirable. In previous methods, the carboxylation reaction required a preformed organometallic reagent to react with CO_2. In this study, we have discovered the hydroalumination of allene derivatives with diisobutylaluminum hydride in the presence of 5 mol % NHC-CuCl without any additive, generating a variety of allyl aluminum reagents, which were directly and regioselectively reacted with carbon dioxide. The desired allylic carboxylic acids were obtained in high yields from mono- and 1,1-disubstituted allenes.

Poster Presentation : **ORGN.P-392**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Copper-Catalyzed Hydroamination of Pyrazole with Oxa/aza-norbornadiene

Kundo Kim, Yunmi Lee[*]

Department of Chemistry, Kwangwoon University, Korea

Bicyclic molecules with oxygen- and nitrogen-containing functional groups are substructures frequently found in biologically active compounds and natural products. Hydroamination using oxa- and aza-bicycloalkenes is a promising way to synthesize the functionalized oxa/aza-bicyclic targets. In particular, pyrazole and its derivatives exhibit a broad range of biological and pharmacological properties, such as analgesic, antifungal, abtidiabetic and antibacterial. Therefore, we developed a new and selective hydroamination of pyrazoles with oxa/aza-norbornadienes promoted by an NHC-Cu catalyst. Our methodology is attractive due to the use of cheap and easy-to-handle copper catalyst, and the use of readily available oxa/aza-norbornadiene as a starting materials. The amination was carried out in the presence of 5-7 mol % NHC-Cu and KOt-Bu under mild reaction conditions, providing various pyrazole-substituted bicyclic products in high yields up to 98% with excellent stereoselectivity.

Poster Presentation : **ORGN.P-393**
Organic Chemistry
Zoom 6 WED 17:30~18:00

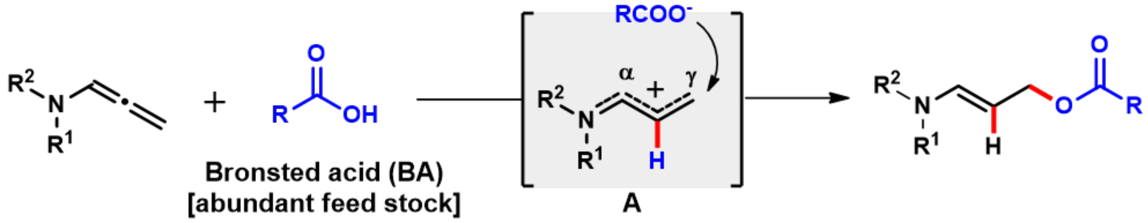
Highly Chemoselective Esterification from *O*-Aminoallylation of Carboxylic Acids; Metal- and Reagent-Free Hydrocarboxylation of Allenamides

Hae Eun Lee, Paul Ha-Yeon Cheong[1,*], Jin Kyoon Park[*]

Department of Chemistry, Pusan National University, Korea
[1]*Department of Chemistry , Oregon State University , United States*

The value of ester groups has been well described by many applications in drug discovery, polymerization, and electronic development.[1] Enamide groups have received particular attention as versatile ambiphilic building blocks for biologically relevant molecules, including therapeutically important natural products and drug molecules.[2] The attractive and unique chemical properties of allenes have attracted many organic synthetic chemists, developing transition-metal catalyzed step- and atom-economic transformation methods. Despite the great and noble success in transition-metal catalyzed chemistry, in terms of greener and sustainability, the demands for developing transition-metal free processes have been growing fast.[3] As a result of our continuous interest and research on the selective transformations of allenamides, we first found the transition-metal free hydrocarboxylation of allenamides by simple BrØnsted acid electrophilic activation of allenamides affording linear ally ester derivatives which could be used for late-stage functionalization and have excellent chemo-, regio-, and stereoselectivity. Furthermore, for the mechanistic investigations, we engaged density functional theory computations. The DFT results revealed that this transformation went through two step mechanism; first protonation which formed iminium-carboxylate and second carboxylation forming the desired hydrocarboxylation product.

Self-activation and mefal-free hydrocarboxylation of allenamide



exogenous reagent-free, broad scope & high yield, late-stage functionalisation

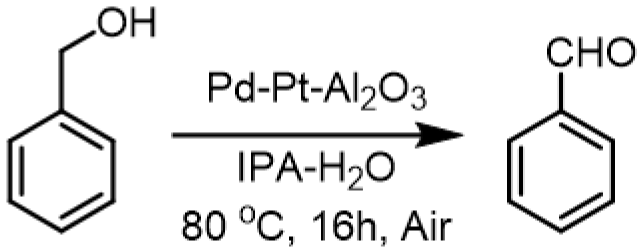
Poster Presentation : **ORGN.P-394**
Organic Chemistry
Zoom 6 WED 17:30~18:00

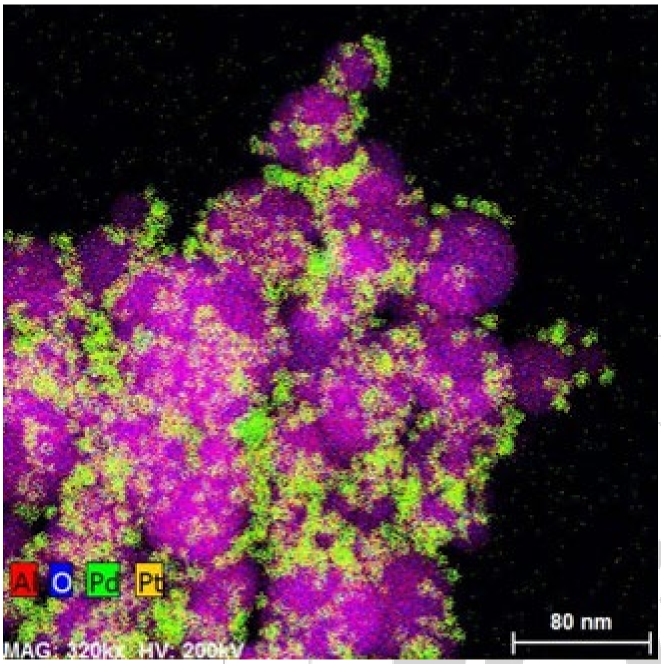
Heterogenous bimetallic Pd-Pt supported on Al_2O_3 as catalyst for benzyl alcohol oxidation under air atmosphere

Lei Cao, Jin Kyoon Park[1,*]

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

A heterogenized catalyst bimetallic Pd-Pt alloy nanoparticles (NPs) supported on Al_2O_3 was synthesized. The Pd-Pt-Al_2O_3 can be easily prepared through a one-pot solution phase hydrothermal method using palladium chloride ($PdCl_2$) and potassium tetrachloroplatinate (K_2PtCl_4) as bimetallic Pd-Pt source with subsequent deposition on the surface of commercial Al_2O_3 nanoparticle. Various characterization results confirmed the generation of Pd-Pt bimetallic alloy, as well as the high dispersion on Al_2O_3 surface. Resulting from the synergistic effect of Pd-Pt bimetallic alloy, the bimetallic Pd-Pt-Al_2O_3 catalyst shows highly selective oxidation property of primary alcohol converting to aldehyde efficiently in air at atmospheric pressure using water and isopropanol cosolvent. Higher conversion and selectivity were achieved over Pd-Pt-Al2O3 comparing with monometallic catalyst Pd-Al_2O_3 or Pt-Al_2O_3. Varity of benzyl alcohol derivatives with electron-withdrawing or electron-donating groups were oxidized to corresponding aldehydes. In addition, the Pd-Pt-Al_2O_3 catalyst can be easily reused up to 7 times without obvious loss of catalytic activity (conversion > 94% and selectivity > 99%).


OH
Pd-Pt-Al2O3
IPA-H2O
80 °C, 16h, Air
CHO


Al
O
Pd
Pt
80 nm
MAG: 320kx HV: 200kV

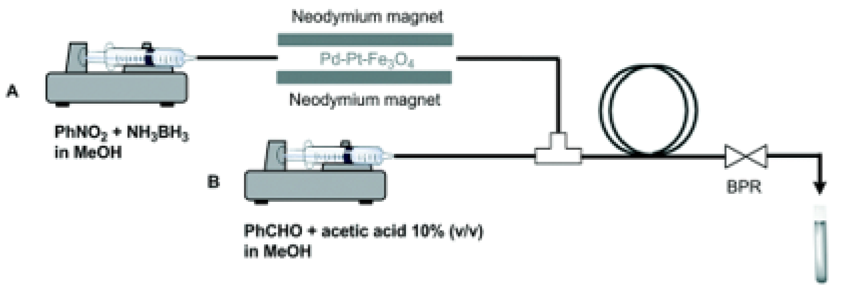
Poster Presentation : **ORGN.P-395**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Simple reversible fixation of a magnetic catalyst in a continuous flow system: ultrafast reduction of nitroarenes and subsequent reductive amination using ammonia borane

Lei Cao, Byeong Moon Kim[1,*], Jin Kyoon Park[2,*]

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

Amination of aldehydes with various nitroarenes forming secondary amines was developed using continuous flow reaction technology. The continuous reaction contains a three-step process of nitro reduction, imine formation, and imine reduction, using Pd-Pt-Fe_3O_4 and NH_3BH_3 as a catalyst and a reductant, respectively. Comparing with previously reported batch-type reactions involving H_2 in high pressure and temperature, the continuous flow reaction was carried out under much more mild condition with room temperature and 40 psi. A variety of secondary amine products were obtained with good to excellent yields (up to 96%). A large range of nitroarenes substituted with electron-donating or electron-withdrawing groups ignoring ortho-, meta- or para- positions could react efficiently with various aromatic or even aliphatic aldehydes substituted with different groups. Moreover, gram scale of product was achieved without much effort by extending the continuous flow progress to 24 h and there was no significant decrease in catalytic property of Pd-Pt-Fe_3O_4 which indicated the potential of industrial application.



Poster Presentation : **ORGN.P-396**
Organic Chemistry
Zoom 6 WED 17:30~18:00

A New Route to Acyl Fluorides via DAST-Mediated Fluorinative Beckmann Fragmentation of Activated Ketones

Danhee Kim, Hee Nam Lim[1,*]

Department of Chemistry, Korea University, Korea
[1]*Eco-Friendly New Materials Research Center, Korea Research Institute of Chemical Technology, Korea*

A new synthetic method of acyl fluorides is presented with a strategy using pull and push-driven Beckmann fragmentation reaction of activated ketones. The previous methods mostly rely on the use of carboxylic acids as starting materials. However, this method features use of α-oximinoketones as substrates. When the substrates were subjected to diethylaminosulfur trifluoride (DAST) derivatives, the corresponding acyl flurorides were obtained with high efficiency, demonstrating our hypothesis of pull and push-driven C-C bond cleavage. The wide availability of the ketones allowed for a broad reaction scope including acylic and cyclic ketones. The developed reaction was highly chemoselective, fast, mild, and efficient.

Poster Presentation : **ORGN.P-397**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Synthesis of new benzorhodamine analogues

Mingchong Dai, Yun Jae Yang[1], Kyo Han Ahn[1,*]

Chemistry, Pohang University of Science and Technology, Korea
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Organic fluorophores with large Stokes shift (>80 nm) are necessary to avoid cross-talk between the excitation and the fluorescent emission in cellular microscopic imaging.[1] Also, some biomolecules cause significant autofluorescence that can be serious interference in tissue imaging. To minimize this issue, the fluorophores emitting in the near-infrared (NIR) wavelength region with large Stoke shifts are great demand for imaging.Rhodamines and its derivatives are well known as suitable organic fluorophore for laser dyes and fluorescent probes due to their properties; high quantum yield, absorption coefficient and photostability.[2] They are widely used in imaging of structure and dynamics of single molecule and micelles in live cell. However, they absorb and emit in short wavelength region below 600 nm and have small Stokes shift. To compensate those drawbacks, we have synthesized new rhodamine analogues with an additional benzene ring in the rhodamine xanthene core forming linear and bent shaped. These modifications lead extension of emitting wavelength region to the orange (~600 nm, bent shaped) and NIR regions (~750 nm, linear shaped) with large Stokes shift in aqueous media. They also have high photostability, optical brightness, absorptivity and good solubility in aqueous media which are ease off those drawbacks of known rhodamine dyes. Based on these new series of benzorhodamine dyes, we expect a new platform of biological application of imaging materials will be provided.[3]References1. J. F. Araneda et al., *Int. Ed.*, **2011**, *50*, 12214−12217.2. H. Zheng et al., *Chem. Commun.*, **2013**, *49*, 429-447. 3. M. Dai et al., *Chem. Eur.J*, **2020**, *26*, 11549 –11557.

Poster Presentation : **ORGN.P-398**
Organic Chemistry
Zoom 6 WED 17:30~18:00

A Light-Emitting Molecular Gear: Correlating, Amplifying, and Transducing Bond-Rotating Motions into Optical Signals

Sungmoon Ji, Dongwhan Lee[*]

Division of Chemistry, Seoul National University, Korea

Artificial rotors and gears are developed to reproduce macroscopic mechanical motions at the molecular scale. When rotatory motions of adjacent chemical bonds are made to correlate, a gear-like molecular device is created. Such conformational transmission can amplify local structural distortion into global conformational change, in a manner reminiscent of protein dynamics of allosteric signaling. To mimic the interdigitation of mechanical gears in a small molecule setting, rigid and rotor components should be placed in close proximity within a sterically congested environment that still allows for free rotation of the axles. In addition, the number of rotating components should be minimized to suppress uncorrelated motions. With these design principles in mind, we have designed and synthesized an overcrowded polyheteroaromatic molecule by installing six propeller-like fragments around a three-fold symmetric core. Constructed with 25 aryl rings, this molecule has only six rotatable bonds, which undergo correlated gear-like motions in the excited-state to produce an exceptionally large Stokes shift. This presentation will discuss key design concepts, synthetic implementations, experimental observations, and mechanistic interpretations.

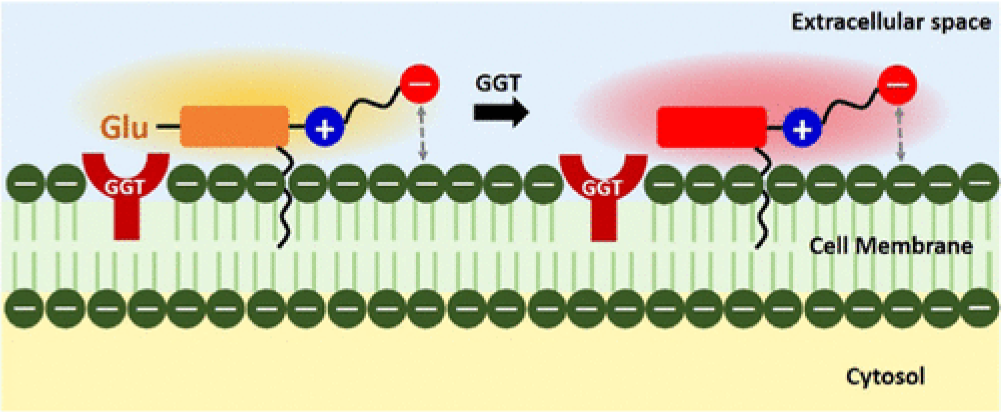
Poster Presentation : **ORGN.P-399**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Cell-Membrane-Localizing, Two-Photon Probe for Ratiometric Imaging of γ-Glutamyl Transpeptidase in Cancerous Cells and Tissues

Yun Lim Jung, Ye Jin Reo, Kyo Han Ahn[*]

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

γ-Glutamyl transpeptidase (GGT) is a cell surface-bound protease which maintains the intracellular glutathione levels and, at its elevated levels, is associated with various diseases including cancer. The detection of the enzyme thus has received much attention, leading to about 40 activatable fluorescent probes so far. All of the known probes, however, lack the membrane-localizing ability, raising a reliability issue in the quantitative analysis. Disclosed is the first fluorescent probe that selectively localizes in the outer cell membrane and detects the enzyme bound there, which, furthermore, is capable of ratiometric as well as two-photon imaging with desirable features. Ratiometric imaging of several cancer and normal cell lines provided quantitative enzyme activity levels, revealing 6.4–8.4-fold higher levels in the case of cancer cell lines than the case of normal cell lines. A comparison of the enzyme activity in organ tissues of normal and tumor xenograft mice reveals notably different levels of enzyme activity depending on the kind of tissue. Normal tissues exhibited comparable levels of enzyme activity, except the kidney that has significantly higher GGT activity (2.7–4.0-fold) than the other organs. Compared with the normal tissues, considerably higher enzyme activity was observed in the tumor tissues of the thigh (4.0-fold), colon (2.5-fold), lung (3.6-fold), and liver (2.1-fold). In contrast, little difference was observed in the enzyme activity between the tumor and normal mice in the case of spleen, stomach, and pancreas tissues. The probe offers practical means for further investigations of GGT-associated biology in cells and tissues by one- as well as two-photon ratiometric imaging.


Extracellular space
Glu
GGT
GGT
GGT
Cell Membrane
Cytosol

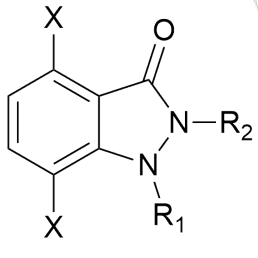
Poster Presentation : **ORGN.P-400**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Synthesis and Biological Evaluation of Indazol-3-one and Indazole derivatives.

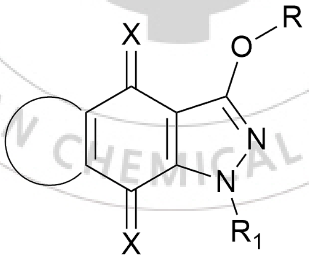
Kyungmin Kim, **Heejae Choi**[1,*], **Hakwon Kim**[*], **Hakwon Kim**[*]

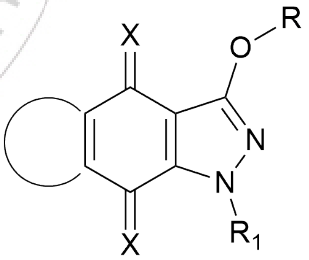
Department of Applied Chemistry, Kyung Hee University, Korea
[1]*Applied Chemistry, Kyung Hee University, Korea*

New indazol-3-one or 3-alkoxyindazole derivatives fused with aromatic compounds, such as benzene, which are expected to be important in terms of biological activity, were synthesized and tested for biological activity. The structures of the isomers of final compound were determined through NMR, MS and X-ray crystallography. In addition, MTT assay and Griess assay were used to investigate the activity of these compounds against inflammation, and the trend between their structure and biological activity was observed.



Indazol-3-one





Poster Presentation : **ORGN.P-401**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Pd-catalyzed selective γ-arylation of aliphatic amines with transient directing groups

Hyeon Bin Ha, HoJeong Choi, Jaesung Kwak[1], Byunghyuck Jung[2], Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea
[1]*Infectious Diseases Therapeutic Research Center, Korea Research Institute of Chemical Technology, Korea*
[2]*School of Basic Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Pd-catalyzed γ-position *sp*^{3}-C-H arylation of primary amines bearing an aliphatic chain or cycloalkyl substituent have been developed with transient directing group (TDG) strategy, and its mechanism has been proposed with computational studies, metalated intermediates, and kinetic isotope effect (KIE) studies. The catalytic development with TDG has been intensively studied for various transformation including C-H bond activations. [1] In this study, 2-hydroxybenzaldehyde derivative plays a key role as a TDG in γ-position *sp*^{3}-C-H arylation to assist the selective and efficient C–H activation of a Pd catalyst. Furthermore, the development of tandem reaction to transform 1^{O}-amines into β-aryl substituted ketones demonstrates the synthetic utilities. Detail catalytic conditions, substrate scopes, DFT calculation for mechanism, X-ray structure of palladacycle compound, and result of KIE study will be discussed during the presentation.

Reference

1. H. Ha, J. Lee, M. H. Park*, B. Jung*, M. Kim. *Bull. Kor. Chem. Soc.* **2020**, *41*, 582.

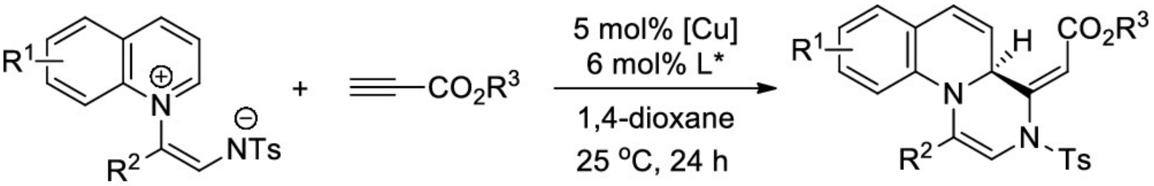
Poster Presentation : **ORGN.P-402**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Cu(I)-Catalyzed Enantioselective [5 + 1] Cycloaddition of N-Aromatic Compounds and Alkynes via Chelating-Assisted 1,2-Dearomative Addition

Donguk Ko, Eun Jeong Yoo*

Department of Applied Chemistry, Kyung Hee University, Korea

[m + n] Cycloadditions are one of the most powerful methods for the construction of polycyclic N-heterocycles which are the core skeletons in enormous number of natural products and biologically active compounds. Especially, the asymmetric hetero Diels-Alder reaction, representative [4 + 2] cycloaddition, is one of the most powerful strategy for optically active six-membered heterocyclic compounds in a single operation. Our group has disclosed that an N-aromatic zwitterion with unusual charge distribution could serve as a five-atom donor, leading to the development of many [5 + n] cycloadditions for medium-sized heterocycles. In this symposium, we will discuss the asymmetric copper-catalyzed [5 + 1] cycloaddition of quinolinium zwitterions and terminal alkynes, resulting in the formation of optically pure six-membered ring systems. The developed cycloaddition to six-membered adducts is characterized by high stereoselectivity and good functional group tolerance, and thus has sufficient potential as a surrogate of asymmetric hetero Diels-Alder reaction.



√ 6-Exo-dig selectivity √ (*E*)-Selectivity √ Enantioselectivity

Poster Presentation : **ORGN.P-403**

Organic Chemistry

Zoom 6 WED 17:30~18:00

To Go Beyond Is as Wrong as To Fall Short: Anion Recognition in Water by Hydrophobicity-Driven and Aggregation-Induced Emission of Multicationic Fluorophores

Soohyung Kim, Jongmin Kim[1], Jongmin Kim[2,*]

Division of Chemistry, Seoul National University, Korea

[1]*Division of chemistry, Seoul National University, Korea*

[2]*Department of chemistry, Seoul National University, Korea*

The recognition of anions in water remains a key challenge in synthetic supramolecular chemistry. Existing strategies usually exploit the reactivity of receptors towards nucleophilic anions, while the detection of inert hydrophobic anions needs to rely on electrostatic interactions. We have devised a modular and readily reconfigurable multicationic molecular scaffold that exhibits aggregation-induced emission (AIE). In water, these molecules display selective fluorescence “turn on” response towards hydrophobic anion. A combination of scanning electron microscope (SEM) and dynamic light scattering (DLS) studies confirmed that such optical response has its origin in the anion-induced aggregation. Detailed structural analysis by X-ray crystallography and NMR spectroscopy revealed that intimate anion–π^+ interactions between the hydrophobic surface of the fluorophore and hydrophobic anion are responsible for this supramolecular phenomenon. We further demonstrated that the inherent hydrophobicity of these anion-responsive molecules can be modulated to achieve higher sensitivity by systematically varying the alkyl pendant chain length. In this presentation will be discussed key design principles, synthetic implementations, and rational strategies to achieve high-sensitivity detection of anion in water.

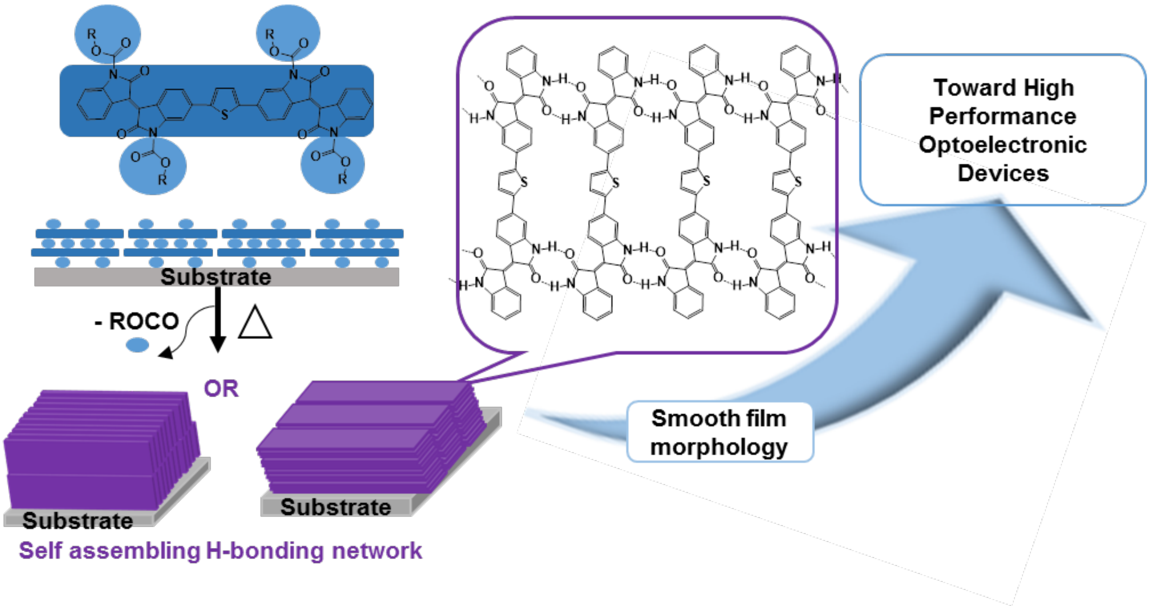
Poster Presentation : **ORGN.P-404**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Molecular organized isoindigo based small molecules with terminal thermally cleavable protecting group

Mohamed Shaker, Hironobu Hayashi[1], Hiroko Yamada[1,*]

Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt
[1]*Division of Materials Science, Graduate School of Science and Technology, Nara Institute of Science and Technology (NAIST), Japan*

The potential of a new series of H-bonded isoindigo (ID) based small molecules as charge transporting materials was examined. The soluble precursor units contained two terminal isoindigo units bearing tert-butoxycarbonyl (Boc) solubilizing substituents. Thiophene, thienothiophene and/or diketo pyrrolopyrrole are used as π-conjugated spacers between the isoindigo units. The protected Boc-ID units are converted to the hydrogen-substituted counterparts by annealing the spin-coated precursor films up to 220 ◦C. The solid state molecular ordering after Boc thermal decarboxylation was investigated using thermogravimetric analysis, UV–vis spectroscopy and X-ray diffraction analysis. The thermogravimetric analysis confirmed the full removal of Boc groups. It was revealed that the formation of terminal intermolecular hydrogen bonds gave the ability to the deprotected materials to change their molecular ordering to edge-on or face-on orientation based on the spacer size and the π-conjugated length. The [-NH——O—C] H-bonding dramatically improved the strength of the intermolecular interactions and induced a significant shift on the wavelength of annealed films. The hole mobilities of isoindigo based organic materials measured by the space charge-limited current (SCLC) method and showed a tenfold improvement after thermal decarboxylation.


Substrate
- ROCO
△
OR
Substrate
Substrate
Self assembling H-bonding network
Smooth film morphology
Toward High Performance Optoelectronic Devices

Poster Presentation : **ORGN.P-405**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Copper-catalyzed asymmetric reduction of α,β-unsaturated lactones using pinacolborane

Lee Soyeon, Jaesook Yun[1,*]

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

Kinetic resolution and dynamic kinetic resolution of α,β-unsaturated lactones were investigated via copper-catalyzed hydroboration using HBpin the presence of amine base. The chiral copper-hydride catalyst reduced the matched unsaturated lactone in excellent diastereo- (99 : 1) and enantioselectivity (99%) in good to moderate yields under epimerization conditions of the starting lactone.

Poster Presentation : **ORGN.P-406**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Cobalt-Catalyzed Defluorosilylation of Aryl Fluorides via Grignard Reagent Formation

Soobin Lim, Hyungdo Cho[1], Jongheon Jeong, Jang Minjae, Hyunseok Kim[2], Seung Hwan Cho, Eunsung Lee*

Department of Chemistry, Pohang University of Science and Technology, Korea
[1]*Division of Chemistry and Chemical Engineering, California Institute of Technology, United States*
[2]*Department of Chemistry, The Scripps Research Institute, United States*

Transition metal-catalyzed transformation of carbon-fluorine bond not only tackles an interesting problem of challenging bond activation, but also offers new synthetic strategies where the relatively inert C–F bond is converted to versatile functional groups. C−F bond functionalization also offers a chance to exploit the prevalent commercial sources of aryl fluorides that comprise more than 30% of the commercially available halogenated arenes, including fluorine-containing drugs. Given these advantages, it is not surprising that continuous efforts done in this area realized successful development of C–C bond-forming reactions, aminations, borylations, and hydrogenations of aryl fluorides.Among them, one particularly interesting transformation is a silylation of aryl fluorides. Organic silanes are widely used in organic electronics, photonics, pharmaceuticals, and polymers. Furthermore, they are important precursors in organic synthesis and can be straightforwardly substituted by various functional groups either via cross-coupling or oxidation. Therefore, several novel defluorosilylation methods of aryl fluorides were recently reported although there was a limited scope of silyl groups.Herein, we report a practical cobalt-catalyzed silylation of aryl fluorides that uses a cheap electrophilic silicon source with magnesium. This method is compatible with various silicon sources and can be operated under aerobic conditions. Mechanistic studies support in situ formation of a Grignard reagent, which is captured by electrophilic silicon sources.

Poster Presentation : **ORGN.P-407**

Organic Chemistry

Zoom 6 WED 17:30~18:00

Copper-catalyzed asymmetric Intramolecular coupling of 1,3-dienes with benz-tethered ketone moieties

Ranjan Acharyya, Soyoung Kim[1], Jaesook Yun[1,*]

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

A straightforward and asymmetric route for the synthesis of biologically active 1,2-dihydronaphthalene-1-ol derivatives were developed using intramolecular copper-catalyzed reductive coupling of easily accessible 1,3-dienes with benz-tethered ketone moieties. This method provided the cyclized products in good yields with excellent enatio- and diastereoselectivities. A six-membered boat-like transition state is proposed for the formation of the major products.

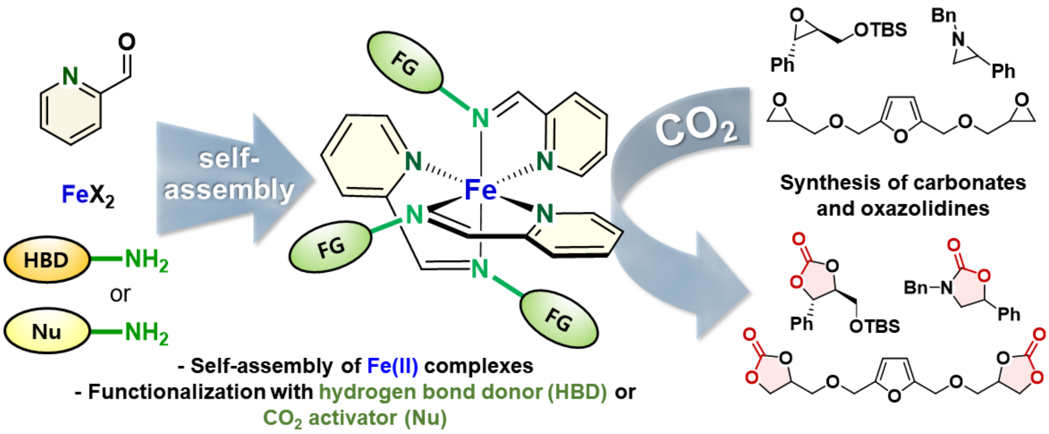
Poster Presentation : **ORGN.P-408**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Self-Assembled Multifunctioanl Fe-Iminopyridine Catalysts and Carbon Dioxide Utilization

Seunghyun Lee, **Jae Hyung Kim**[1], **Eun Joo Kang**[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Although it has recently been recognized that global supplies of the most useful metal ores are being exhausted, Fe remains one of the five most abundant metals in the Earth’s crust. The development of Fe catalysts for the large-scale production of cyclic carbonates is a meaningful investigation. Our sustainable Fe-iminopyridine catalyst systems were investigated for the formation of cyclic carbonates or oxazolidinones from carbon dioxide and epoxides or aziridines, respectively, under mild conditions (50 °C, 3 bar CO_2). The homoleptic and heteroleptic Fe catalysts were prepared by a convenient self-assembly protocol. The optimal catalyst contained a hydrogen bond donor to activate substrate ring opening and a nucleophilic imidazole group to activate the CO_2 electrophile. This approach represents a green CO_2 recycling method to afford value-added chemicals with potential industrial applications. A wide range of cyclic carbonates and oxazolidinones was synthesized in excellent yield and selectivity under mild conditions. Thus, this approach represents a green CO_2 recycling process for producing valuable chemicals with potential industrial applications. Further investigations on carbon utilization and the recycling of carbon dioxide are underway as valuable sources of useful chemicals and eco-friendly materials.


O
N
FeX$_2$
HBD
NH$_2$
or
Nu
NH$_2$
self-assembly
FG
N
N
Fe
N
N
N
N
FG
FG
CO$_2$
O
OTBS
Ph
Bn
N
Ph
O
O
O
O
O
Synthesis of carbonates and oxazolidines
O
O
O
Ph
OTBS
O
Bn–N
O
Ph
O
O
O
O
O
O
O
O
O
- Self-assembly of Fe(II) complexes
- Functionalization with hydrogen bond donor (HBD) or CO$_2$ activator (Nu)

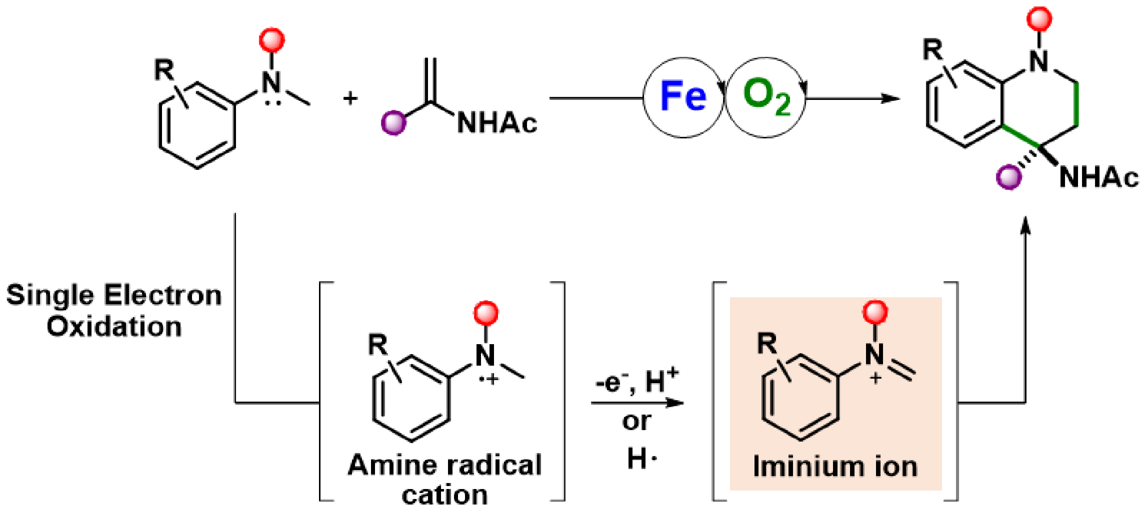
Poster Presentation : **ORGN.P-409**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Iron-Catalyzed [4+2] Cycloaddition Reactions of Tertiary Anilines with Electron-Rich Olefins under Aerobic Condition

Duyong Park, Joon Young Hwang[1], Eun Joo Kang[1,*]

Department of Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Oxidative transformation of tertiary amines generates nucleophilic α-aminoalkyl radical, which can be oxidized to electrophilic iminium ion by single-electron oxidation process with transition metal catalysts (Ru, Ir, Ni, and Cu). Iminium ion can react with nucleophilic reaction partners such as indole, nitromethane, phenylacetylene, and enamide. In 2016, Guan group reported dehydrogenative [4+2] cycloaddition reaction of tertiary anilines with enamides by $FeCl_3$ and tert-butyl hydrogenperoxide (TBHP) catalytic system for the synthesis of tetrahydroquinolines with quaternary carbon centers. However, it is important to develop methodology having green chemical reaction condition. Recently, our research group reported redox-selective α-amino functionalization with electron-deficient olefins by aerobic catalytic system of $[Fe(phen)_3(PF_6)_3]$ complex. Herein, we report α-amino functionalization of tertiary anilines with electron-rich olefins using iron polypyridyl complex under aerobic condition. This research presents a broad range of product from simple tetrahydroquinolines to complex skeletons such as julolidine, phenothiazine derivatives.


R
N
+
NHAc
Fe
O2
R
N
NHAc
Single Electron Oxidation
R
N
Amine radical cation
-e-, H+
or
H·
R
N
+
Iminium ion

Poster Presentation : **ORGN.P-410**

Organic Chemistry

Zoom 6 WED 17:30~18:00

Investigation of Intramolecular Cyclization of Dienyl Substituted Acetophenones Using Copper Complexes

<u>Wanseok Yoon</u>, Jaesook Yun[*]

Department of Chemistry, Sungkyunkwan University, Korea

A stereodivergent synthesis of functionalized dihydroindenols and dihydronaphthalenols by copper-catalyzed intramolecular cyclization of dienyl substituted acetophenones was developed. Depending on the ligand used (NHC vs. bisphosphine), the same starting material resulted 5-membered or 6-membered cyclized product, respectively. In case of dihydronaphthalenols, enantiomerically enriched dihydronaphthalenols were obtained in good yields and ee values up to 93 % with a chiral ligand.

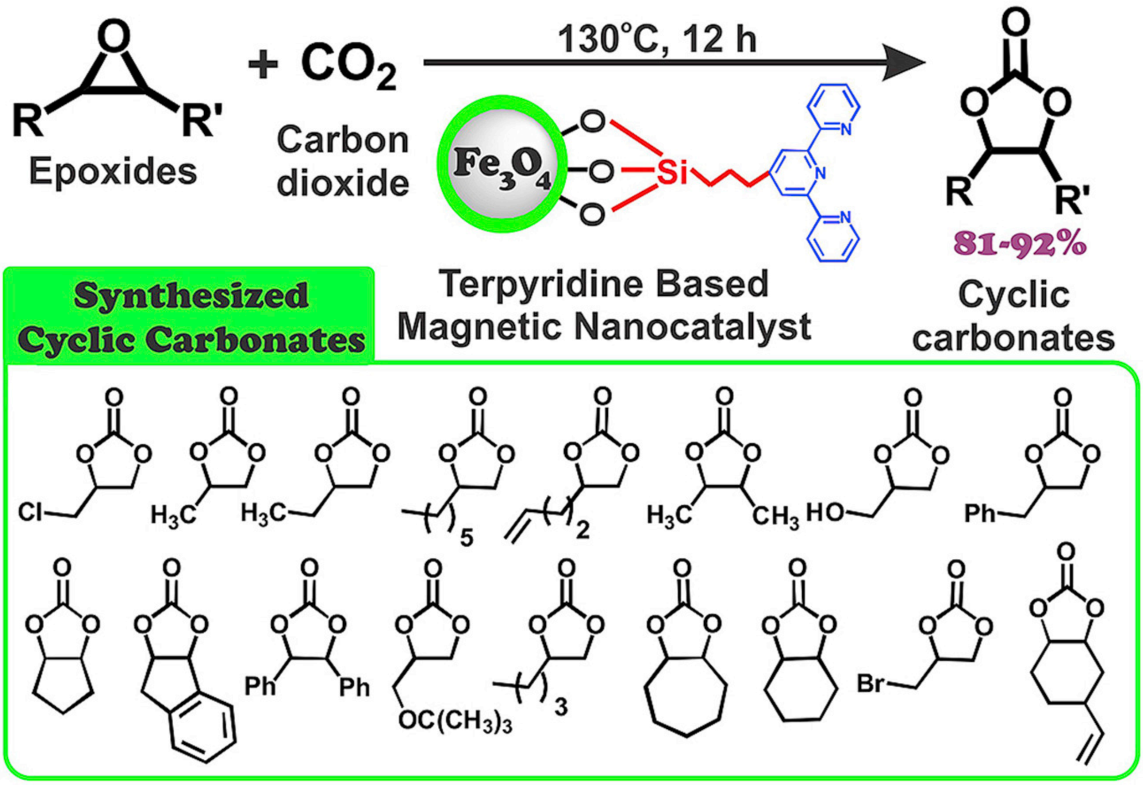
Poster Presentation : **ORGN.P-411**
Organic Chemistry
Zoom 6 WED 17:30~18:00

Terpyridine-Pr-Fe3O4@boehmite nanoparticles; a novel and highly effective magnetic nanocatalyst for preparation of cyclic carbonates from carbon dioxide and epoxides under solventless conditions

Faisal Muhammad, Aamer Saeed[*]

Organic chemistry, Quaid-i-Azam University, Pakistan

In this research work, moisture- and air-stable terpyridine-mediated magnetic boehmite (terpyridine-Pr-Fe3O4@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, N2 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-Fe3O4@boehmite nanoparticles were applied as nano-catalyst for the synthesis of cycliccarbonates form the cycloaddition coupling reaction of carbon dioxide with epoxides under solvent-less conditions. The cost-effective nano-catalyst 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 there action 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
O
Si
N
Terpyridine Based Magnetic Nanocatalyst
81-92%
Cyclic carbonates
Synthesized Cyclic Carbonates
Cl
H3C
HO
Ph
CH3
5
2
3
OC(CH3)3
Br

Poster Presentation : **ORGN.P-331**

Organic Chemistry

Zoom 7 WED 16:30~17:00

Diarylpyrazine-based position isomers: A detailed study of optical properties and structure property relationship

Dong Jin Park, Young Dae Gong[1,*]

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

A versatile synthetic route to pyrazine-based symmetrical and unsymmetrical D-A flanked chromophores has been designed to study their structural effects on optical properties. Suzuki-Miyaura coupling of dihalopyrazine with various aryl boronic acids was synthesized under microwave condition. Pyrazine functionalized at C-2, C-5 and C-6 served as π-bridge or acceptor to construct linear and angular push-pull chromophores. The photophysical, electrochemical as well as thermal properties of these linear and angular chromophores were investigated and results were correlated theoretically by density functional theory computations. The permutation of terminal donor acceptor units tunes the optoelectronic properties in a predictable way, aiding in the rational design of small molecule for luminescent materials. These chromophores displayed multicolor change in different solvents, exhibiting good solvatochromism with a large stokes shift.

Poster Presentation : **ORGN.P-332**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Facile Direct Synthesis of *N*-Aryl-Substituted Azacycles from *N*-ethyl protected Arylamines via $TiCl_4$-Mediated Reaction

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

N-Substituted azacycles are widely observed in bioactive small molecules and pharmaceuticals including FDA-approved clinical drugs. Thus, some synthetic method using primary amines have been used to prepare useful azacycles. However, reaction of alkyl arylamines, secondary amines, were rarely carried to produce azacycles due to low activity of alkyl arylamines. We are desirable to discover novel direct preparation of *N*-aryl substituted azacycles from *N*-alkyl arylamines. Thus, in this study, several Lewis acid reagents and bases were tested to give direct conversion of *N*-ethyl arylamines to *N*-aryl substituted azacycles, and it was found that $TiCl_4$ was useful reagents for the reaction with cyclic ethers, and DBU was suitable partner base. Specially, utilization of combined reagents, $TiCl_4$ and DBU, in this reaction could readily afforded *N*-substituted azacyles. Particularly, a series of five- and six-membered azacycles were synthesized in high yield. The combined Lewis acid and base mediated method can be a promising direct synthetic protocol to prepare *N*-aryl substituted azacycles from *N*- ethyl arylamines.

Poster Presentation : **ORGN.P-333**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Direct $AlCl_3$-Catalyzed Transformation of THP Protected Alcohols

Tien Tan Bui, Hee-Kwon Kim[*]

Department of Nuclear Medicine, Jeonbuk National University, Korea

Tetrahydropyranyl (THP) groups are commonly utilized as protecting group of alcohols in the form of tetrahydropyranyl ethers because THP ethers are chemically stable and easily prepared from various alcohols. Both direct conversion of THP protected alcohols to azides and direct nucleophilic substitutions of THP protected alcohols by carbon nucleophiles are useful organic chemistry. In this study, several catalysts and azide reagents were examined for the transformation of benzyl THP ethers, and it was found that $AlCl_3$ and $TMSN_3$ were suitable reagents to perform direct conversion of benzyl THP ethers to azido compounds. Using synthetic method, various benzyl THP ethers was successfully reacted with $TMSN_3$ in the presence of $AlCl_3$ produce azido compounds in high yield. In additions. direct nucleophile additions of carbon nucleophiles to benzyl THP ethers in the presence of catalytic $AlCl_3$ to form C-C bond was readily achieved under mild reaction condition. The results suggest that this novel method could be used to various direct transformations of THP protected alcohols such as azidation, allylation, and alkynylation

Poster Presentation : **ORGN.P-334**
Organic Chemistry
Zoom 7 WED 16:30~17:00

The Direct Conversion of *N*-Cbz-Protected Amines to Ureas using Lanthanum (III) Trifluoromethanesulfonate

Tien Tan Bui, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Because ureas have been found in valuable applications in many areas such as organic materials and natural products, several preparations of ureas have been used. However, traditional synthetic methods have drawbacks including instability of intermediates or hazardous nature of reagent such as phosgene. Usually many amines have been protected by Cbz protecting group in organic syntheses due to generation of unwanted side products. Therefore, development of novel preparation method of urea from *N*-Cbz-protected amines is valuable study. In this study, various triflate salts were examined for direct conversion of *N*-Cbz-protected amines to urea compounds, and then it was found that lanthanum trifluoromethanesulfonate was the most suitable catalyst for this direct reaction. Additionally, urea compounds were successfully prepared when reaction was carried out in $PhCF_3$ as a solvent. Using the lanthanum trifluoromethanesulfonate catalyzed reactions conditions, reactions of Cbz-carbamates originating from various aromatic and aliphatic amines with numerous amines readily yielded the corresponding ureas in great transformation yield. The result presented that the direct preparation of ureas from *N*-Cbz-protected amines in the presence of lanthanum trifluoromethanesulfonate is a highly efficient method.

Poster Presentation : **ORGN.P-335**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Synthesis and Evaluation of Novel Multivalent Fluorescent Translocator Protein Ligand for Glioma Cancer

Tien Tan Bui, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

The 18kDa translocator protein (TSPO) is defined as one class of peripheral benzodiazepine receptor which is related to a wide array of biological metabolism. Recently, TSPO has been developed as attractive biological target for both diagnosis and therapeutics in oncology due to its overexpression in several types of cancer. Therefore, several imaging agents bearing specific TSPO ligand structure have been studied for better diagnostic purpose. In this study, novel multivalent TSPO ligand bearing *N*-(2-hydroxybenzyl)-*N*-(4-phenoxypyridin-3-yl)acetamide scaffolds with an optical probe was designed. The core TSPO ligand structure was synthesized from 4-chloro-3-nitropyridine as a starting material. *N*-(Carbobenzyloxy)-L-glutamic acid was employed to give dimeric structure, and SCy5.5, a NIR fluorescence probe, was introduced to dimeric TSPO ligands. Novel multivalent flurorescent TSPO ligand was evaluated in an animal model of glioma cancer, and it was found that novel TSPO imaging agents have shown intense signal and high contrast at the tumor region compared to normal region. These results suggest the novel multivalent fluorescent TSPO ligand could be a promising diagnostic agent for cancers.

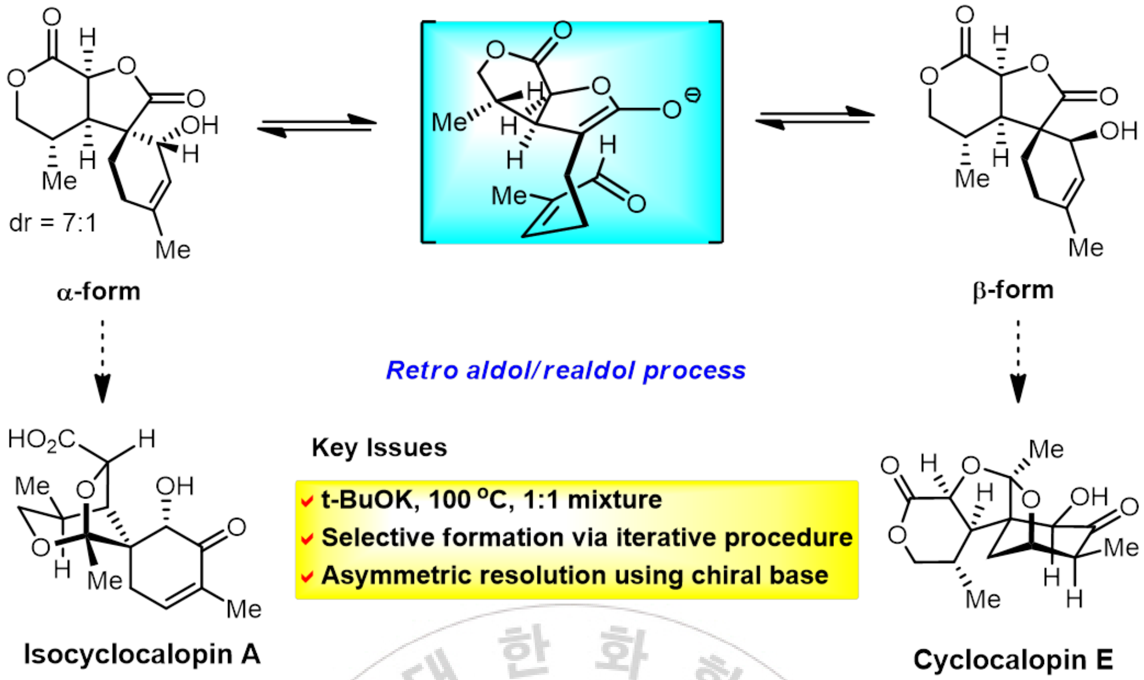
Poster Presentation : **ORGN.P-336**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Equilibrium of Spirosystem in Cyclocalopin via Retroaldol/Realdol Process: Selective Formation of alpha- or beta-epimer via Iterative Procedure

Jieun Song, **Jimin Kim**[*], **Chan-Mo Yu**[1,*]

Department of Chemistry, Chonnam National University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. Recently, we have developed reaction routes from allenyl glyoxylate to bicycliclactone in 3 step sequence. In order to construct a spirosystem in cyclocalopin natural products, cycloaddition of bis-lactone with diene provided adducts in a ratio of 7:1. However, both epimers have been existed in nature. Is it possible to obtain alpha or beta form selectively? 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 in cyclocalopin structure via retro- and re-aldol process. ii. Selective formation of alpha- or beta-form via iterative equilibrium procedure. iii. Toward a synthesis of cyclocalopin A.



Key Issues

- t-BuOK, 100 °C, 1:1 mixture
- Selective formation via iterative procedure
- Asymmetric resolution using chiral base

Poster Presentation : **ORGN.P-337**

Organic Chemistry

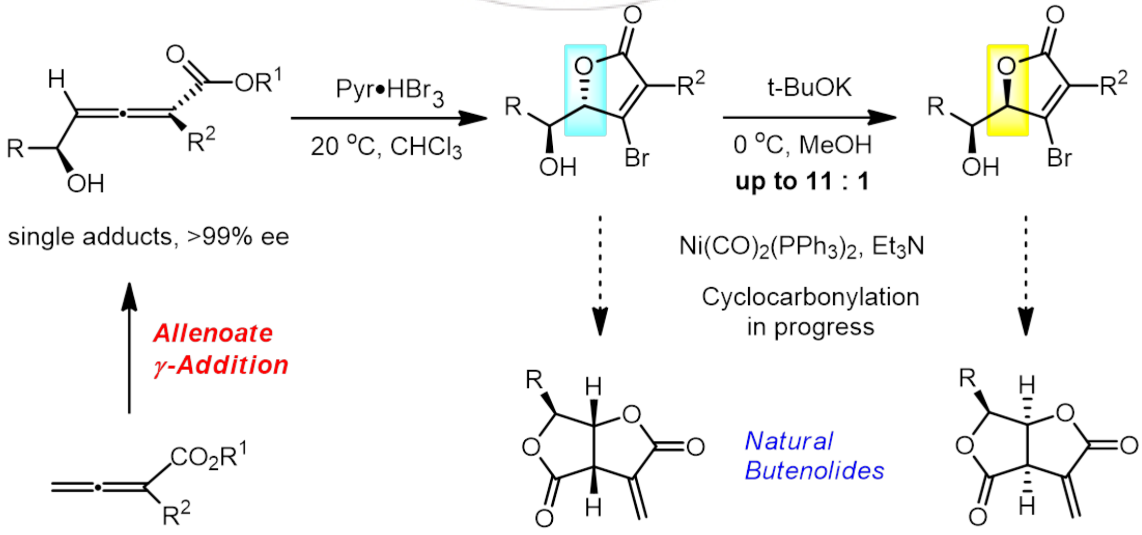
Zoom 7 WED 16:30~17:00

A Conversion of erythro-5-(4-bromo-1-hydroxyakyl)-furan-2(5H)-ones to threo-Diastereomers under Basic Conditions: Origin of Thermodynamic Stability

Euijin Park, Jimin Kim[*]

Department of Chemistry, Chonnam National University, Korea

During the past two decades, substantial progress has been made for a variety of stereoselective methods mediated by chiral reagents and catalysts. Nevertheless, only a limited number of methods exist to construct both diastereomers selectively, despite their plentiful synthetic potential. Recently, we have disclosed a new method for the stereospecific synthesis of furanone derivatives via two step sequence: asymmetric allnoate gama-addition followed by regiospecific cyclization via gold catalysis or bromination as described below. During the investigations, we experienced that gamma-lactone moiety was sensitive to epimerize under basic conditions. Consequently, we speculated that erythro isomer can be converted to the corresponding threo-diastereomer. We would like to present herein reaction conditions, scope and limitation of the reaction, and its synthetic applications to bioactive substances.



Poster Presentation : **ORGN.P-338**

Organic Chemistry

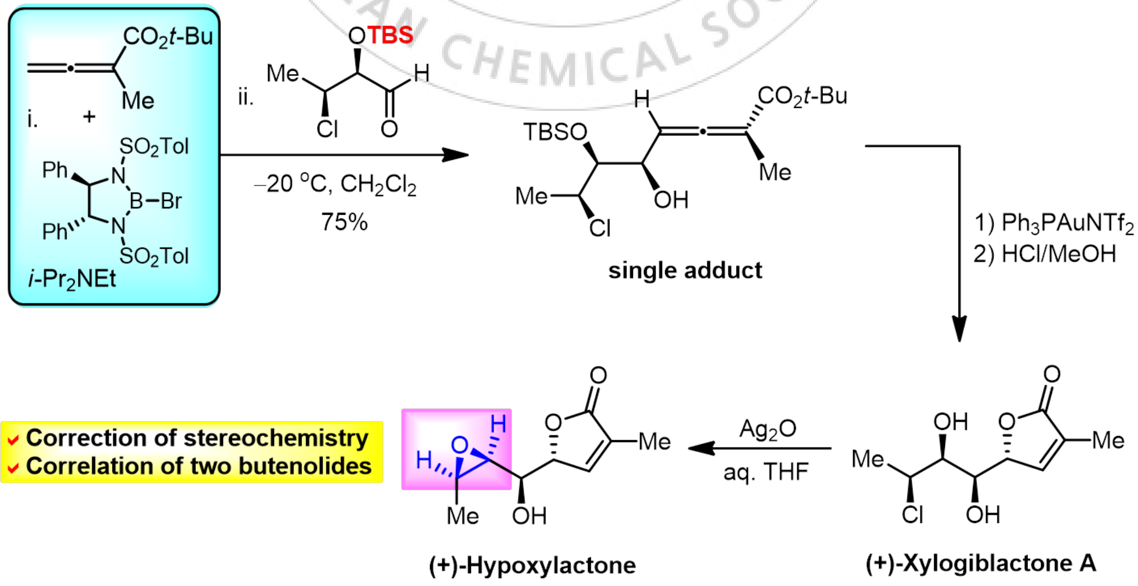
Zoom 7 WED 16:30~17:00

Synthesis of Naturally Occurring (+)-Hypoxylactone and (+)-Xylogiblactone A: Correction and Verification of Stereochemistry

Sehui Yang, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. Among a variety of synthetic methods for the Synthesis of natural gamma-lactone polyketide (+)-hypoxylactone has been achieved in four-step sequence for the first time. This highly stereoselective synthesis of (+)-hypoxylactone involves three major key transformations: i) highly stereoselective allenoate gamma-addition of aldehydes to provide only single adduct. ii) regiospecific cyclization of gamma-adducts through gold catalysis to provide gamma-lactone unit. iii) epoxidation of a chlorohydrin functionality using Ag_2O to yield the cis epoxide for (+)-hypoxylactone without any epimerization of gamma-lactone ring. This investigation led to the correction and verification of the known relative and absolute stereochemistry.



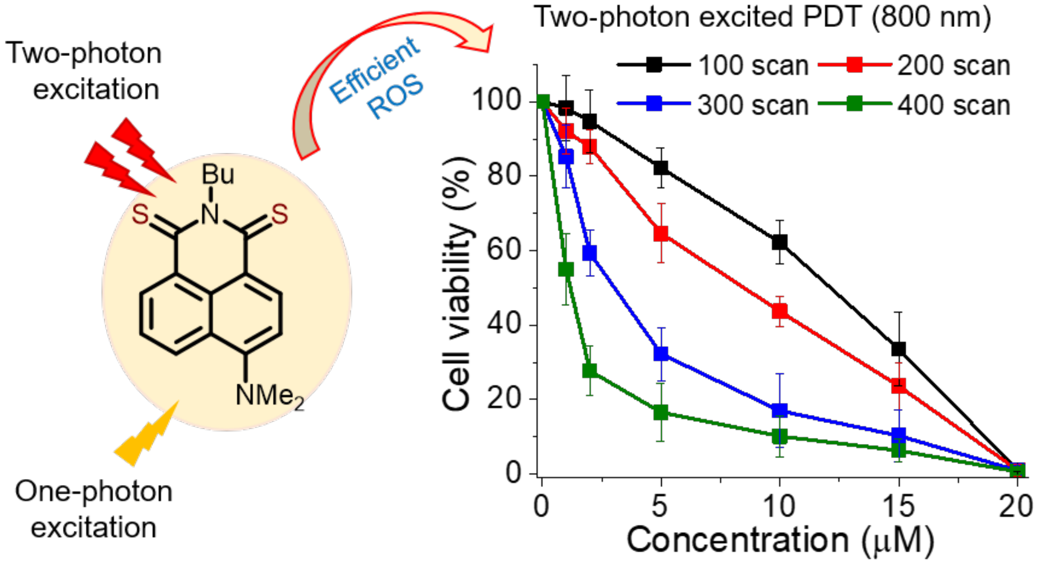
Poster Presentation : **ORGN.P-339**
Organic Chemistry
Zoom 7 WED 16:30~17:00

The development of heavy-atom-free photosensitizers for two-photon excited photodynamic cancer therapy

Jeongsun Ha, Seon Ye Heo, Sujie Qi, DongJoon Lee[1], Hwan Myung Kim[1,*], Juyoung Yoon[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Department of Energy Systems Research, Ajou University, Korea*

Photodynamic therapy has been widely used to treat malignant diseases. However, it has not reached its full potential. This is partly due to a lack of efficient photosensitizers and the limited depth of tissue penetration by visible light. In this study, a series of thiocarbonyl compounds (NIS and CRNS) were developed as novel photosensitizers for photodynamic cancer therapy without the use of heavy atoms. Replacing oxygen atoms in conventional naphthalimide and coumarin derivatives with sulfur atoms was essential for enhancing intersystem crossing (ISC), which led to near-unity singlet oxygen quantum yields in air-saturated organic solutions. Interestingly, under two-photon excitation, NIS-Me and CRNS demonstrated excellent ROS generation capability in both aqueous solutions and cancer cells. The photosensitizers also displayed good biocompatibility and low dark toxicity in living cells. In particular, the phototoxicity of NIS-Me and CRNS towards HeLa cells and HeLa spheroids was outstanding upon two-photon excitation at 800 nm, providing deep insight for the molecular design of photosensitizers based on sulfur-substituted carbonyl fluorophores.


Two-photon
excitation
Bu
N
S
S
NMe$_2$
One-photon
excitation
Efficient
ROS
Two-photon excited PDT (800 nm)
100 scan
200 scan
300 scan
400 scan
Cell viability (%)
0
20
40
60
80
100
0
5
10
15
20
Concentration (μM)

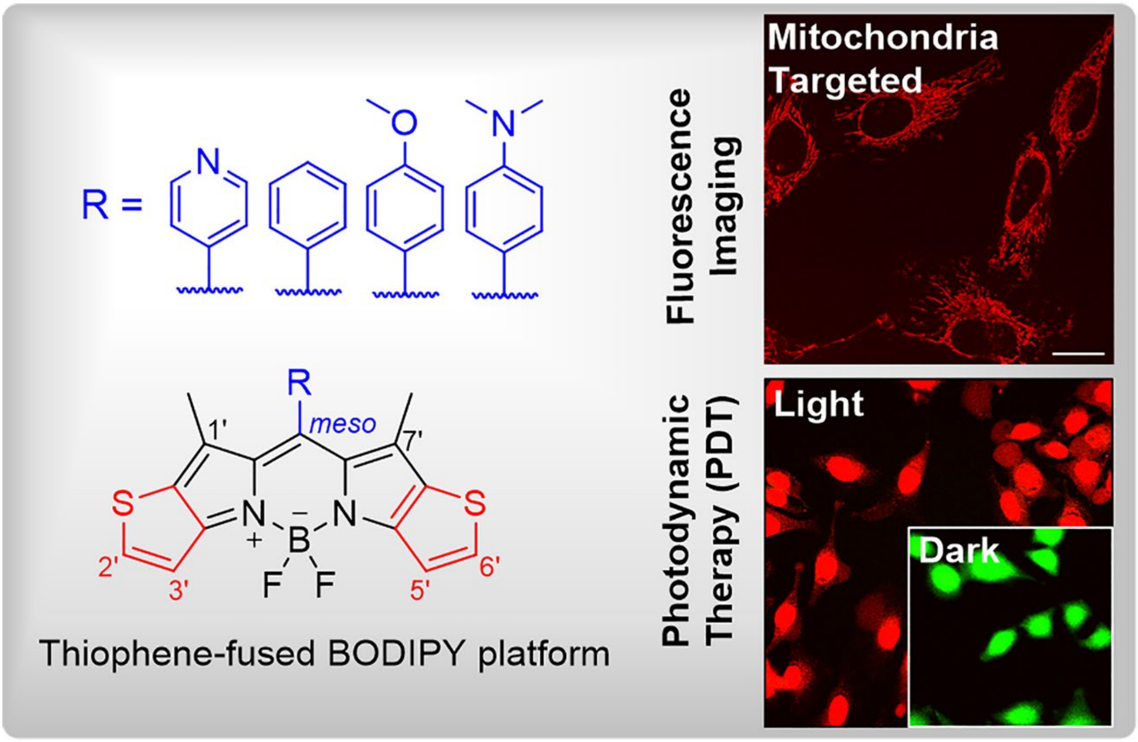
Poster Presentation : **ORGN.P-340**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Fine-tuning the electronic structure of heavy-atom-free BODIPY photosensitizers for fluorescence imaging-targeted photodynamic therapy

Sujie Qi, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Theranostics that integrates diagnosis into therapy platform has received great attention as an effective approach for cancer treatment. However, the engineering of efficient theranostic agents with excellent optical properties for the clinic still is a challenge. Herein, we designed novel heavy-atom-free BODIPY photosensitizers (R-BODs) that possess strong $^1O_2$ generation abilities and good fluorescence properties for imaging-guided photodynamic therapy (PDT). The sulfur atoms fusing into the π-conjugated skeleton of BODIPY along with the introduction of different functional groups to the meso-site of the BODIPY core is essential for tuning the photophysical and photochemical properties. In particular, the MeOPh-substituted thiophene-fused BODIPY (MeO-BOD, R = p-methoxyphenyl) displayed the highest $^1O_2$ generation capability ($\Phi_\Delta \approx 0.85$ in air-saturated acetonitrile) and a moderate fluorescence quantum yield (Φ_f = 17.11%). The MeO-BOD NPs showed good biocompatibility, low dark toxicity, and superior fluorescence imaging properties in living cells. Moreover, the PDT efficacy of mitochondria-specific anchoring of MeO-BOD was remarkably enhanced with a very low half-maximal inhibitory concentration (IC_{50}) value of 95 nM. The incorporation of an electron-donating group at the meso-position of the thiophene-fused BODIPY platform will provide an approach to develop the effective theranostic agents for precision cancer therapy.


R =
N
O
N
R
meso
1'
7'
S
S
N
N
B
+
−
F
F
2'
3'
5'
6'
Thiophene-fused BODIPY platform
Fluorescence Imaging
Mitochondria Targeted
Photodynamic Therapy (PDT)
Light
Dark

Poster Presentation : **ORGN.P-341**

Organic Chemistry

Zoom 7 WED 16:30~17:00

A benzothiazole-based fluorescent chemosensor for detecting Cu^{2+} in aqueous media

Seon Min Park, Doo OK Jang*

Department of Chemistry, Yonsei University, Korea

Studies on chemosensors that recognize cations are important. The needs for the recognition of metal cations have been increased, because they have harmful effects on health of human and the environment.We designed and synthesized a benzothiazole derivative with pyridine moiety to optically detect cations. It was expected that the unshared electrons of nitrogen and sulfur atoms in the receptor could recognize cations. The receptor recognized Cu^{2+} ions selectively even in the presence of other metal ions. After addition of Cu^{2+} ions, the fluorescence intensity of emission band at 456 nm increased in aqueous media. The binding stoichiometry between receptor and Cu^{2+} were determined 1:1 through job's plot analysis.

Poster Presentation : **ORGN.P-342**
Organic Chemistry
Zoom 7 WED 16:30~17:00

A Microenvironment-Sensitive Fluorene-Labeled 2'-Deoxyuridine as a Probe to Detect the Presence of an DNA Abasic Site

Seung Woo Hong, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

In this study, we found that the fluorene-labeled 2'-deoxyuridine (**U^F^**) displayed sensitive fluorescent properties, showing a large fluorescence change depending on the polarity and viscosity of the solvent. This environment-sensitive $\mathbf{U^F}$ was incorporated into the central position of oligodeoxynucleotide (ODN) and different flanking bases (FBs) were placed around the $\mathbf{U^F}$ in order to investigate whether the fluorescence change was observed when the ODN probes containing $\mathbf{U^F}$ met the abasic site. Among them, the ODN probe containing cytosine-FBs turned on fluorescence for the target DNA with fully matched sequences, while dramatically turned off fluorescence for the target DNA having an abasic site.

126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **ORGN.P-343**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Copper-Catalyzed Oxidative C-C Cleavage

Siae Kim, Seong Eon Kim, Hye-Young Jang[1,*]

Department of Energy System Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

The conversion of biopolymer into useful chemicals is the sustainable and valuable chemical process. Lignin is a type of biopolymer and is composed of aromatic compounds. Therefore, investigating catalytic systems converting lignin-derived compounds into aromatic compounds is being actively conducted. Most studies specifically focus on the C-C and C-O bonds cleavage in lignin-derived compounds using a variety of catalysts. In our study, we report selective copper-catalyzed C-C bond cleavage using lignin-derived compounds (1,2 diol and 1,3 diol) to aldehydes. Mechanism studies explain the reaction route of C-C bond cleavage and formation of aldehydes without over oxidation. Therefore, this study will guide a direction to convert lignin-derived compounds into value-added aromatic compounds through a copper catalytic system.

Poster Presentation : **ORGN.P-344**

Organic Chemistry

Zoom 7 WED 16:30~17:00

Design and synthesis of dinitropyrazole-based high energy materials

Byeongil Lee, Young gyu Kim*, Kuktae Kwon[1], SeungHee Kim[1]

Division of Chemical & Biological Engineering, Seoul National University, Korea
[1]*Agency for Defense Development, Korea*

Explosive performances of high energetic materials (HEMs) are influenced mostly by their molecular structure, density, heat of formation and oxygen balance. As their explosive performances increase, however, so does the sensitivity of the HEMs to various external stimuli in most cases, making the development of HEMs with high explosive performance and low sensitivity difficult to put into practice. For that reason, there have been many synthetic and computational studies of HEMs that would have high performances and low sensitivity. Pyrazoles are a kind of azoles having five-membered nitrogen-containing heterocyclic compounds and known to have aromaticity and high heat of formations. Because of their stable chemical properties, nitro-substituted pyrazoles are promising building blocks in HEMs chemistry. Herein, we will present some nitrated pyrazole structures as a basic skeleton for promising HEMs and their efficient synthetic ways via coupling reactions with their characterization results.

Poster Presentation : **ORGN.P-345**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Development of Efficient and Safe Nitration Methods for Pyrazole Derivatives via Flow Chemistry

Se Won Bae

Department of Chemistry, Jeju National University, Korea

The military continues to be interested in the development of Insensitive Munitions while maintaining the effectiveness of the High Explosive composition. Most of nitration reactions for the synthesis of molecular explosives are currently being synthesized through Batch Chemistry (BC). However, nitration reaction through BC has sometimes shown problems in safety, scalability, and generates large amounts of synthetic by-products, resulting in low economic efficiency and environmental issues. Accordingly, there is an urgent need for a more safe, cost-effective and eco-friendly synthesis method that can replace BC. Flow Chemistry (FC) is emerging as a new synthetic platform to replace BC because of its ease of scale-up, easy yield improvement, low synthetic by-products and the ability to perform the synthesis process very safely. The FC process is also attracting attention as a new alternative for developing new synthesis methods that were not possible in BC because of their excellent heat transfer capabilities. This study introduces nitration methods for pyrazole derivatives using FC process.

Poster Presentation : **ORGN.P-346**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Highly luminescent green and yellow OLED for Triazine-dibenzocarbazole based bipolar host materials

Keunhwa Kim, Subin Oh, Han-Su Hwang, Younghee Park, Kyu Yun Chai[1,*], Kanthasamy Raagulan

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

In this study, the following bipolar host materials such as, 7-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-7H-dibenzo[a, g]carbazole (TRZ-DBC1) and 7-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-7H-dibenzo[a, i]carbazole (TRZ-DBC2) were successfully synthesized between dibenzocarbazole donor and triazine acceptor. The TRZ-DBC1 and TRZ-DBC2 exhibited exceptional thermal stabilities and good bipolar features. The yellow and green phosphorescent OLED devices have been fabricated for the study of host performances. The yellow device (TRZ-DBC1) disclosed 71.4 cd/A of outstanding current efficiency, and corresponding reference device (CBP) possessed lower efficiency of 58.0 cd/A. The external quantum efficiency of TRZ-DBC1, TRZ-DBC2, and reference device were 25.4%, 25.4%, 19.1%, respectively. The TRZ-DBC2 with 2.71 eV of higher triplet energy utilized as host material for green phosphorescent OLED and showed excellent current efficiency of 75.9 cd/A, and excellent external quantum efficiency of 24.7 %. Thus, both bipolar host materials can be exploited for green and yellow phosphorescent OLEDs for display application.

Poster Presentation : **ORGN.P-347**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Thermally stable hole transporting carbazole-triphenylamine for red phosphorescent OLEDs

Younghee Park, Keunhwa Kim, Subin Oh, Han-Su Hwang, Kanthasamy Raagulan, Kyu Yun Chai[1,*]

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

In this work, different hole transporting materials with carbazole and triphenylamine have been successfully synthesized. The end capping strategy is used to compare the overall performance of the device for which 3 and 6 position of carbazole is utilized. The materials without crystallized aspect displayed only 5% of thermal decomposition until 500 °C and possess excellent thermal stability. The HOMO energy of the synthesized materials lies in the range of −5.62 - −5.48 eV, while LUMO is positioned between −2.51 - −2.31 eV. The effective hole transportation exist as HOMO value are lying between energy of anode and emission layer. Further, the recombination is facilitated in the middle layer as LUMO is placed within the adjacent layer value (-(2.31-2.51) eV). The triphenylamine based HTMs (2A and 2B) exhibited excellent performances than carbazole based HTMs (1A and 1B) and comparison has been made by using NPB as hole transporting reference material with the same red phosphorescent based OLED device. HTM 2A based device IV was displayed 30.6 cd/A of maximum current efficiency with higher maximum external quantum efficiency of 26.7% than NPB based device. The HTM 2A gave rise hole mobility of 5.3 × 10−4 cm2 V−1 s−1, which was higher than that of NPB. Hence, the HTM 2A is the excellent candidate for thermally stable red OLED applications.

Poster Presentation : **ORGN.P-348**

Organic Chemistry

Zoom 7 WED 16:30~17:00

Boron Lewis Acid-Catalyzed Hydrophosphinylation of N-Heteroaryl Substituted Alkenes with Secondary Phosphine Oxides

Sarah Yunmi Lee*, Jongwon Kim[1]

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

We report herein the first boron Lewis acid-catalyzed process for the hydrophosphinylation of N-heteroaryl-substituted alkenes with secondary phosphine oxides. This reaction proceeds under mild conditions and enables an introduction of a phosphorous atom to alkenylazaarenes with diverse substitution patterns. The available mechanistic data can be explained by a reaction pathway wherein the C–P bond is created by the reaction between the activated alkene (coordinated to a borane catalyst) and the phosphorous(III) nucleophile (in the tautomeric equilibrium with secondary phosphine oxide).

Poster Presentation : **ORGN.P-349**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Photoluminescent and Electrochemiluminescent GSH Sensors Using Cyclometalated Iridium(III) Complexes Based on Different Response Mechanism

Hyun seung No, Jong-in Hong[1,*]

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

Glutathione(GSH) is one of the most important reducing agent in biological system which consists of glycine, cysteine, glutamate. GSH is involved in cellular processes, including cell differentiation, proliferation, and apoptosis. Decreased concentration of GSH leads to an increased susceptibility to oxidative stress implicated in the progression of cancer. So, it is necessary to develop point-of-care (POC) sensors measuring real-time concentration of GSH. Here, we synthesized three cyclometalated Iridium complexes incorporating 1,10-phenanthroline-5,6-dione in auxiliary ligand as a recognition site for GSH which can be detected by photoluminescence and electrochemiluminescence. The di-carbonyl group is reduced to di-hydroxyl group by GSH and the sensors showed turn-on response to photoluminescence and turn-off response for electrochemiluminescence. To elucidate the different response mechanism, we conducted cyclic voltammetry, differential pulse voltammetry and density functional theory studies. It was found that di-carbonyl moiety provides non-radiative pathway which is responsible for the low PL intensity, while lower LUMO energy level of the sensors was attributed to high ECL intensity due to efficient electron transfer from TPrA radical. Further experimental details and results will be presented in the poster section.

Poster Presentation : **ORGN.P-350**
Organic Chemistry
Zoom 7 WED 16:30~17:00

Fluorene-Labeled 2'-Deoxyuridines with Different Linkers: Application as Probes for DNA Duplex Formation

Su Jin Yang, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

Three fluorene-labeled 2′-deoxyuridines that differ in terms of their linkers— **U**$^{\mathbf{F}}$ (without linker), **U**$^{\mathbf{FL}}$ (with ethynyl linker), and **U**$^{\mathbf{DF}}$ (with diethynyl linker)—have been introduced at the central positions of oligodeoxynucleotides to examine the effects that their linkers have on the fluorescence emission properties upon duplex formation with fully matched and single-base-mismatched targets. Here, we describe the influence of the linkers on the emission behavior, the intramolecular electron transfer between the fluorene moiety and the uracil base after photoexcitation, and the structural stability upon duplex formation. The probe containing the **U**$^{\mathbf{FL}}$ residue (with an ethynyl linker) and cytosine residues as flanking bases exhibited the greatest fluorescence turn-on selective behavior toward the perfectly matched target.

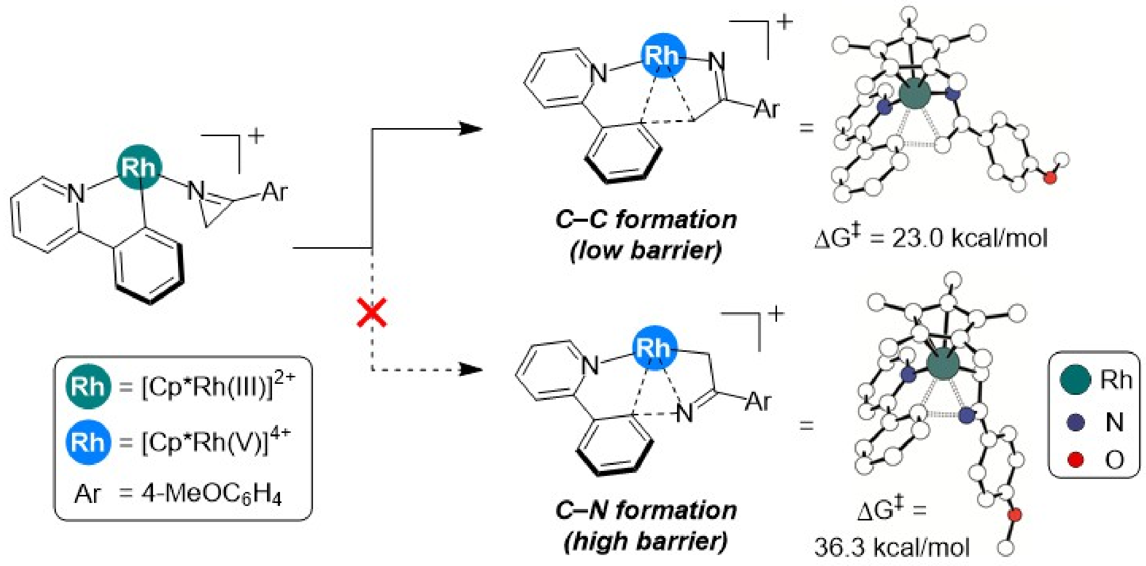
Poster Presentation : **ORGN.P-371**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Selective C–C Bond Formation from Rh(III)-Catalyzed C–H Activation Reaction of 2-Arylpyridines with 3-Aryl-2H-Azirines

Eunseo Lee, Tae Hyeon Kim, Hee Chan Noh, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

A novel method for the synthesis of acylmethyl-substituted 2-arylpyridine derivatives using 3-aryl-2H-azirines was developed by exploring a prototype reaction using DFT-calculations and carrying out targeted experiments guided by the calculated mechanism. 2H-Azirine was initially hypothesized to ring-open at the metal center to furnish familiar metal nitrene complexes that may undergo C–N coupling. Computational studies quickly revealed and prototype experimental work confirmed that neither the formation of the expected metal nitrene complexes nor the C–N coupling were viable. Instead, azirine ring-opening followed by C–C coupling was found to be much more favorable to give imines that readily underwent hydrolysis in aqueous conditions to form acylmethyl-substituted products. This new method was highly versatile and selective toward a wide range of substrates with high functional group tolerance. The utility of the new method is demonstrated by a convenient one-pot synthesis of biologically relevant heterocycles such as pyridoisoindole and pyridoisoqunolinone.


Rh = [Cp*Rh(III)]$^{2+}$
Rh = [Cp*Rh(V)]$^{4+}$
Ar = 4-MeOC$_6$H$_4$
C–C formation
(low barrier)
ΔG‡ = 23.0 kcal/mol
C–N formation
(high barrier)
ΔG‡ =
36.3 kcal/mol
Rh
N
O

Poster Presentation : **ORGN.P-372**

Organic Chemistry

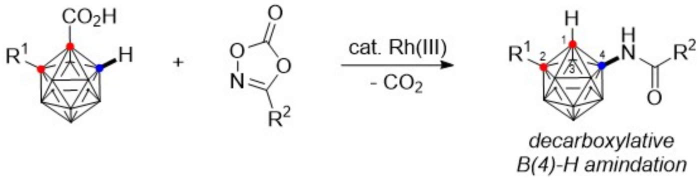
Zoom 7 WED 17:00~17:30

Rhodium(III) Amidation of the Cage B(4)−H Bond in o-Carboranes with Dioxazolones by Carboxylic Acid-Assisted B(4)−H Bond Activation

Hyeongcheol Ham, Eunseo Lee, Phil Ho Lee[*]

Department of Chemistry, Kangwon National University, Korea

Because carboranes, which are a kind of three-dimensional cluster of benzene, have been increasingly investigated as boron neutron capture therapy (BNCT) agents in medicine, as versatile ligands for transition metals, and as building blocks in nanomaterials, introduction of functional groups into carborane clusters has received great attention. To date, a variety of approaches have been reported for the introduction of functional groups into CH and BH vertices of carborane clusters. Nitrogen-substituted carborane clusters have garnered significant attention over the past several years owing to their potential applications in drug and catalyst discovery. For instance, carborane clusters containing nucleoside or amino acid moieties have been used as biological active compounds for tumor treatment in BNCT In addition, ocarborane clusters containing an aminoalkyl group have been largely utilized as ligands in organometallic chemistry. Stimulated by the recent progress in catalytic C−H amination and amidation and the distinctive function of weakly coordinating carboxylic acid as the directing group in regioselective B−H bond activation on carboranes, we have demonstrated rhodium-catalyzed direct and regioselective amidation as well as diamidation of ocarborane with dioxazolones by carboxylic acid-assisted B(4)−H bond activation in carborane clusters.



- ☑ *Rh(III)-catalyzed B(4)-H amidation of o-carborane*
- ☑ *dioxazolones as the nitrogen source*
- ☑ *CO_2 byproduct*
- ☑ *broad substrate scope*
- ☑ *high yields*

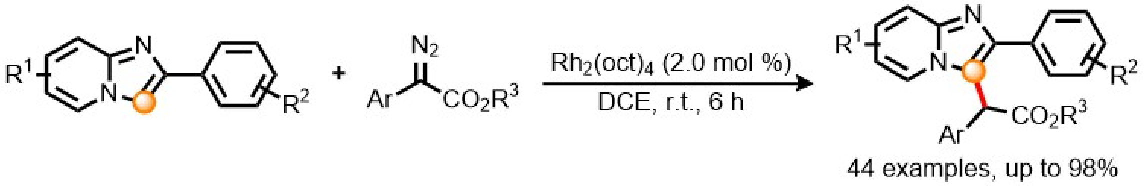
Poster Presentation : **ORGN.P-373**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Rh(II)-Catalyzed Regioselective C3-Alkylation of 2-Arylimidazo[1,2-a]pyridine Derivatives with Aryl Diazoesters

Hee Jin Yang, Hyeongcheol Ham, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Imidazo[1,2-a]pyridines are significant privileged scaf-folds in azaheterocycle chemistry,[1] and they are commonly found in natural products, pharmaceuticals, and biologically active compounds. Among azaheterocycles, imidazopyridines and espe-cially 3-alkyl-2-arylimidazo[1,2-a]pyridines are not only essential pharmacophores but also practical synthetic intermediates that can be easily converted into valuable molecules. A regioselective C3-alkylation based on the reaction of 2-arylimidazo[1,2-a]pyridines with a wide range of aryl α-diazoesters in the presence of a Rh(II) catalyst in dichloroethane at room temperature was developed. This method could be applied in the synthesis of benzoimidazoquinolizinone and cyclo-heptaimidazopyridinone, which are novel heterocyclic scaffolds.



Poster Presentation : **ORGN.P-374**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Micelles-based fluorescence sensor for selective and sensitive detection of transferrin concentration in human serum.

Seoyoon Kim, Seoung Ho Lee[1,*]

Department of chemistry, Daegu University, Korea
[1]*Department of Chemistry, Daegu University, Korea*

Iron is involved in a variety of biological processes within the body, such as electron transport, DNA synthesis, red blood cell production, or even cell division. The monitoring of transferrin that regulates the concentration of iron (III) ion in the body can assess the ability to transport iron (III) ion in the blood. Therefore, it is necessary to sensitively monitor abnormal levels of transferrin in our blood system. In this work, we have devised the novel micellized fluorescence probe complexed with Fe^{3+} ions for sensitive detection of transferrin. The quenched fluorescence of micellized probe by Fe^{3+} ions exhibits increased fluorescence in the presence of apo-transferrin, where strong affinity between apo-transferrin and Fe^{3+} ions induces the decomplexation of Fe^{3+} ions from the micellized probe.

Poster Presentation : **ORGN.P-375**

Organic Chemistry

Zoom 7 WED 17:00~17:30

A fluorescent probe based on micellization of amphiphilic fluorophores derivatives for highly selective and sensitive detection of heparin in human serum

Seung yeob Lee, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Detection of Heparin in human serum is difficult due to the presence of biological obstructions like proteins and lipids. Thus, it is highly challenging to selectively and sensitively detect heparin at the nanomolar concentration level in human serum. Herein, we report micelle-based sensing approach to efficiently detect heparin in human serum. The amphiphilic building block (**1**), consisting of a hydrophobic pyrene unit and a hydrophilic imidazolium salt, displays self-assembly in aqueous media. The aggregated pyrene units at the core serve as a conduit for energy and electron transport, which induces amplified fluorescence quenching for heparin detection. The Stern-Volmer (SV) quenching constant for the fluorescence quenching of micelle-based sensors by heparin is approximately 1.8 X 10^8 M^{-1}. This system can detect heparin levels below nanomolar concentrations in practical conditions.

Poster Presentation : **ORGN.P-376**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Sequential 1,3-*N*- to *C*- and 1,3-*C*- to *C*-Migration of Sulfonyl Groups via the Synthesis of 1,4-Diazepines from the Aza-[5 + 2] Cycloaddition of Indoloazomethine Ylides

HanJoong Kim, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Recently, we found the sequential 1,3-N- to C- and 1,3-C- to C-migration of sulfonyl groups through the synthesis of 1,4- diazepines from the aza-[5 + 2] cycloaddition reaction of indoloazomethine ylides with dialkyl acetylenedicarboxylate. To the best of our knowledge, this migration is unprecedented because the alkyl- and aryl-sulfonyl groups have shifted from the 1-nitrogen atom to the faraway 6-carbon atom. Herein, we have demonstrated the sequential 1,3-N- to C- and 1,3-C- to Cmigration of sulfonyl groups from an operationally simple thermal aza-[5 + 2] cycloaddition reaction of indoloazomethine ylides with dialkyl acetylenedicarboxylates under mild conditions, leading to the formation of C-sulfonylated 1,4- diazepines.
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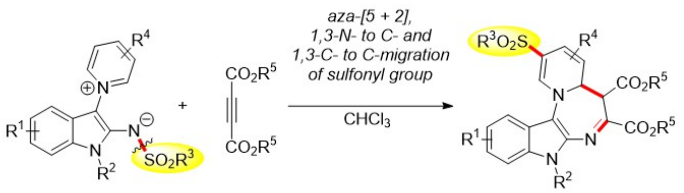


☑ *novel scaffold*
☑ *concise one-pot protocol*
☑ *metal- and additive-free*
☑ *simple operation*
☑ *mild thermal conditions*
☑ *high regioselectivity*

Poster Presentation : **ORGN.P-377**

Organic Chemistry

Zoom 7 WED 17:00~17:30

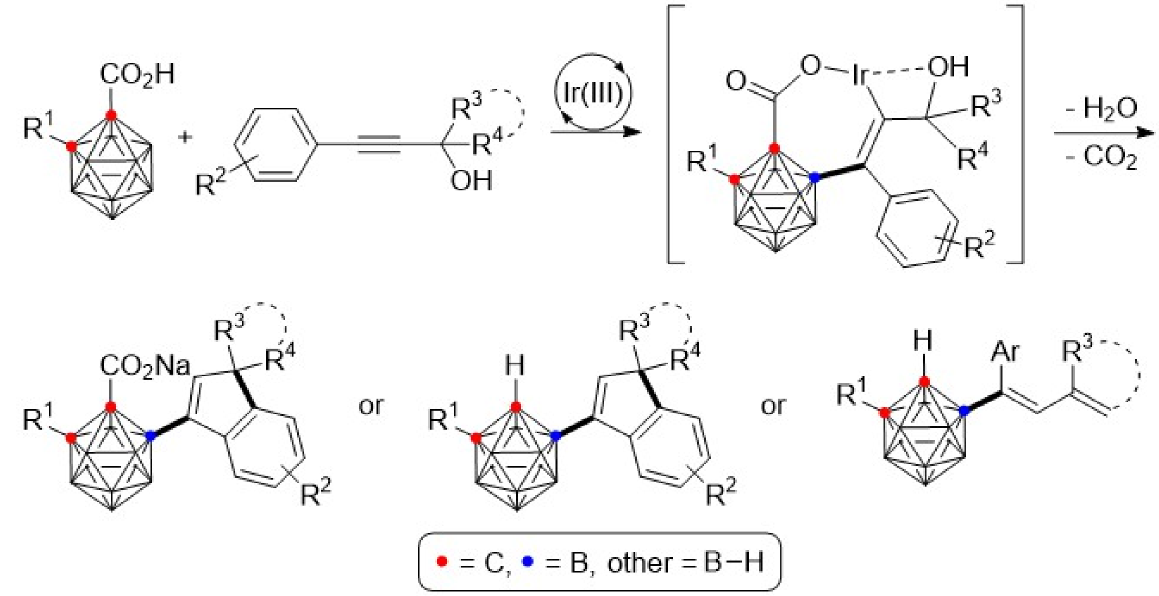
Ir-Catalyzed Cyclative Indenylation and Dienylation via Sequential B(4)−C Bond Formation, Cyclization, and Elimination from o-Carboranes and Propargyl Alcohols

Hee Chan Noh, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Carboranes, which are recognized as a type of threedimensional kindred form of benzene, have found a number of applications in boron neutron capture therapy (BNCT) as medication, in organometallic and coordination chemistry as novel ligands, and in supramolecular design and materials as building blocks. However, the distinctive structures of carboranes make their derivatization laborious, which results in a restricted application range. Therefore, it is highly required to develop new synthetic methods for the functionalization of carboranes. We have developed an iridium-catalyzed cyclative indenylation through B(4)−C bond formation followed by intramolecular C−C bond formation via dehydrative intramolecular electrophilic aromatic cyclization from the reaction of o-carborane with a variety of propargyl alcohols, affording B(4)-indenylated o-carboranes with excellent regioselectivity. In addition, the iridium-catalyzed regioselective 1,3-dienylation has been achieved through sequential B−H activation, dehydration, and decarboxylation, producing B(4)-dienylated o-carborane derivatives. Further studies on the synthetic applications and mechanistic details are currently underway.

B−H activation / Cyclative indenylation / Decarboxylation or B−H activation / Dienylation in o-carborane cluster



Poster Presentation : **ORGN.P-378**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Micelle-based fluorescent probe for efficient detection of dopamine in human serum

HyeBin Song, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Dopamine is an important neurotransmitter for central nervous system function. The abnormal dopamine level causes physiological problem such as Parkinson’s disease, Huntington’s disease and Schizophrenia. Thus, it is important to selectively and sensitively sense the dopamine concentration in human serum. In this work, we have newly designed the pyrene derivative with a phenyl boronic acid (PBA), which forms micelles in aqueous media, as an efficient fluorescence sensor for dopamine detection. The PBA unit selectively recognizes dopamine by formation of boronate-catechol interaction between PBA and dopamine, resulting in amplified fluorescence quenching with a very high Stern-Volmer quenching constant.

Poster Presentation : **ORGN.P-379**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Aggregation-Induced Emission based turn-on probe Tetrazine-Kaleidolizine

Sang-Kee Choi, Seulbi Lee, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Indolizine based fluorophore Kaleidolizine(KIz) is known as tuning the emission wavelength by changing its substituents. The KIz can offer a clear view with low background signal, and an increased signal-to-noise (S/N) ratio, which is ideal for biosensing and bioimaging because of its property of Aggregation-Induced Emission(AIE). Additionally, the well-known fluorescent quencher tetrazine is applied as the substituent of KIz to act both as a reactive handle and quencher moiety. Tetrazine is having attention with its fast and chemoselective [4+2] cycloaddition with specific dienophiles such as Trans-cyclooctene(TCO) without any catalysts. With high selective 'tagging' of specific targets, which is called click chemistry[1], it can provide a means to image or track the components and interactions. As the quenched fluorophore, the tetrazine-modified KIz implies with various application methods by lowering the background signal to enhance the turn-on ratio.

Poster Presentation : **ORGN.P-380**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Development of a Kaleidoscopic fluorescent sensor array for pH sensing

Hyungi Kim, Jun-Sik Min[1], Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

[1]*Molecular science and technology, Ajou University, Korea*

Sensors using fluorescent with high sensitivity and selectivity are attracting attention in variety of research directions. The understanding of structure photophysical relationship of a given fluorophore and development of supramolecular chemistry has enabled the discovery of several useful fluorescent sensors through the integration of chelators or functional moiety at specific position. Here we present a fluorescent sensor array for pH sensing system. Based on pKa value of the functional group, we designed 30 different fluorescent compounds responding with the pH changes via incorporation of pH sensitive functional groups on C-1 position of Kaleidolizine. Simple spotting of the fluorescent compounds on cellulose filter paper printed with wax allowed us to generate a single array. By analyzing fluorescence pattern changes of the array, we successfully monitored the pH differences of the samples.

Poster Presentation : **ORGN.P-381**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Enantioselective Methallylation and Allylation Reaction of Aldehydes with Silane Compounds Catalyzed by a Chiral Lewis Acid

Hye-Min Jeong

Department of Chemistry, Sungkyunkwan University, Korea

The methallylation and allylation reactions of carbonyl compounds are one of the best ways to form carbon-carbon bonds. In our methods, the aromatic and aliphatic aldehydes react with allylsilane under Lewis acid catalyst, COBI (Chiral oxazaborolidinium ion) catalyst to produce homoallylic alcohols. The enantiomeric pure homoallylic alcohols can be used as the chiral building block of various biomolecules. In the presence of COBI catalyst, the reaction proceeded in high yields (up to 99%) with excellent enantioselectivities (up to 99% ee), even without metal reagents. Silane compounds have the advantage of non-toxic, high thermal stability, and rather low sensitivity to moisture and oxygen. A number of applications of this method to various other challenging chemical intermediates and biological active compounds are possible.

Poster Presentation : **ORGN.P-382**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Simultaneous and visual detection of cysteamine based on Michael addition reaction with polydiacetylenes

<u>Seongman Lee</u>, Thanh Chung Pham, Songyi Lee[1,*]

Department of Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

We report fabrication of a highly sensitive colorimetric and fluorometric sensor comprising a self-assembled polydiacetylene (PDA) liposome for the measurement of cysteamine concentration. N-maleimidomethanol (HM) moiety was used as Michael addition acceptor, which reacts with the thiol groups in cysteamine to generate maleimide-thiol conjugation resulting in conformational transition of the conjugated backbone. Further, this chemosensor system displays a clear blue-to-red colorimetric transition in the presence of cysteamine among various biothiols with high selectivity and sensitivity owing to the the structural specificity of Cysteamine.The resulting PDA solutions were analyzed via FE-SEM, UV-vis, fluorescence and Raman spectroscopies, and chromoisomerism for naked-eye visualization. This chemosensor provides a convenient method for the detection of cysteamine in aquatic solution and in real samples.

Poster Presentation : **ORGN.P-383**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Visual Simultaneous Detection of Cadmium Ion Based on Conjugated Polydiacetylenes

Yongkyun Kim, Chaeeon Bae, Yeong Hwan Choi, Sumin Jeon, Songyi Lee[1,*]

Department of Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

heavy metals accumulate in air, water, and soil, and they are not biodegradable. Sensitive and selective detection and quantitation of toxic heavy metals plays a key role in the control of heavy metal pollution. Among these toxic heavy metals, cadmium was listed as a priority substance in the field of water policy by Directive 2008/105/EC of the European Union Parliament and of the European Council on environmental quality standards. In the list, cadmium was identified as a priority hazardous substance. In this regard, considerable effort has been devoted to developing methods for the detection of heavy metals for industrial processes and environmental monitoring. However, the standard and traditional techniques for the analysis of traces of Cd2+ require costly analytical techniques, such as atomic absorption spectrometry (AAS), inductively cou-pled plasma mass spectrometry (ICP-MS), fluorescent sensors, and colorimetric assays. Many fluorescent sensors for cadmium have been reported in past years. However, only a few probes have displayed high selectivity to cadmium over zinc, due to their similarity in physical and chemical properties; they are in the same group of the periodic table. Thus there is a great need for developing Cd2+-selective sensors that can distinguish Cd2+ from Zn2+ with high sensitivity and selectivity under physiological conditions. In the current study, we prepared monomer PCDA-MP, then polymerized them to form polydiacetylene (PDA)-based sensor (PDA-MP), which displayed selective colorimetric and fluorometric change in the presence of cadmium ion (Cd2+) in aqueous solution. The PDA-MP polymer showed colorimetric change from blue to red (violet) in response to various amounts of Cd2+. The chemosensor also exhibited rapid fluorescence turn-on response and significant selectivity to Cd2+ compared with other metallic cations. Naked-eye detection of Cd2+ is accomplished in aqueous solution through PDA-based sensor system.

Poster Presentation : **ORGN.P-384**
Organic Chemistry
Zoom 7 WED 17:00~17:30

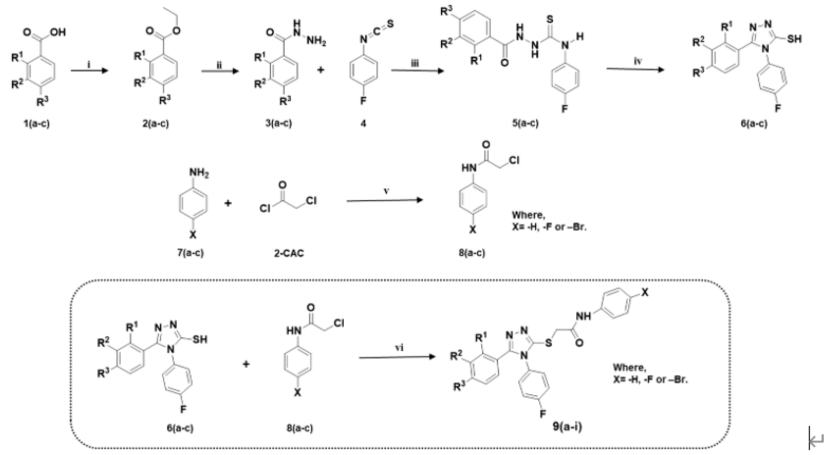
Synthesis of Triazole based derivatives as Tyrosinase Inhibitors: Lineweaver–Burk Plot Evaluation and Computational Ascriptions

Balasaheb Daniyal Vanjare, Nam Gyu Choi, Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

Novel tyrosinase inhibitors were synthesized through multistep reaction pathway and their structures were examined by spectral techniques including FT-IR, 1H NMR and 13C NMR. The enzyme inhibition effects of these tyrosinase inhibitors were evaluated and kinetics mechanism was analysed by Lineweaver–Burk plots. The binding profile of these molecules were ascribed through molecular docking studies. These synthesized molecules were identified as potent inhibitors relative to the standard (kojic acid) and 9h inhibited the tyrosinase non-competitively by forming an enzyme-inhibitor complex. The inhibition constant Ki (0.018 μM) for 9h was calculated from Dixon plots. Docking results also displayed that all compounds possessed good binding profile against tyrosinase and interacted with core residues of target protein.

Synthesis scheme:



Scheme 1: Synthesis route, reagents and conditions: i) ethanol, Conc. H2SO4 , reflux; ii) hydrazine hydrate (NH2-NH2), ethanol, reflux; iii) ethanol, ambient temperature, 12 h; iv) H2O, 2N NaOH, 70-80°C, v) triethylamine, dichloromethane; vi) Potassium carbonate, dimethylformate (DMF), ambient temperature, 4-5 h.

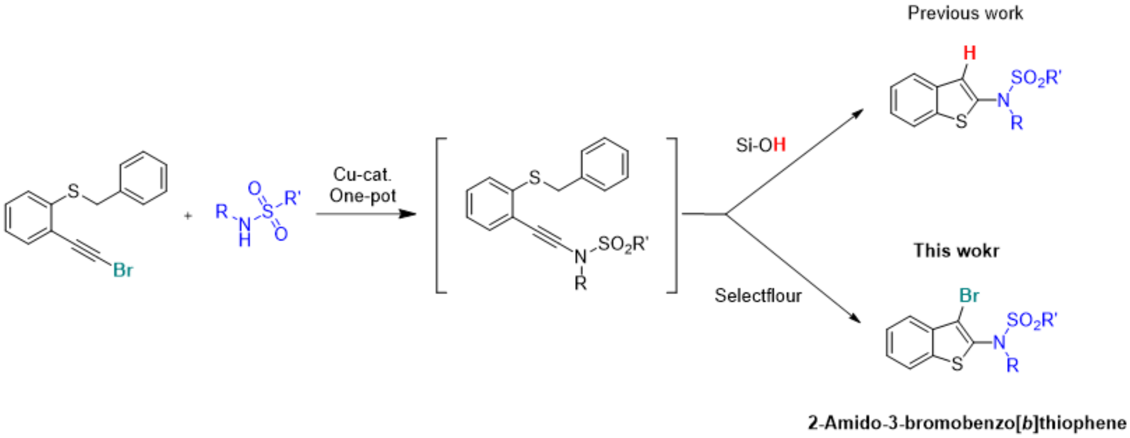
Poster Presentation : **ORGN.P-385**
Organic Chemistry
Zoom 7 WED 17:00~17:30

A Selectfluor promoted Cu-catalyzed One-Pot Synthesis of 2-Amido-3-bromobenzo[b]thiophene from Bromoalkyne

ChangJu Yoon, Do Hyun Ryu[1,*], Hyun Suk Yeom[2,*]

Sungkyunkwan University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*
[2]*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

Benzo[*b*]thiophenes are naturally occurring heterocyclic compounds with diverse applications in medicinal chemistry and material science, resulting in high interest in industry as well as academia. Thus, the synthesis of muti-substituted benzo[*b*]thiophenes has attracted great attention over the past few decades; a number of synthetic routes for 2,3-disubstituted benzo[*b*]thiophenes through intra- and intermolecular reactions have been reported. In particular, 3-bromo benzo[*b*]thiophene is an important intermediate to introduce aromatic substituents at the 3-position. In most cases, stoichiometric amount of bromination reagents (NBS, and Br_2) or $CuBr_2$ have been required for the halocyclization of alkyne.Recently, we reported the silica-gel assisted synthesis of 2-amido benzo[*b*]thiophenes from the corresponding (o-thioanisole) substituted ynamides. This high reactivity of ynamide was expected to enable effecient synthesis of 3-substituted-2-amidobenzo[*b*]thiophene through reaction with suitable electrophile. Therefore, in order to introduce F at 3-position, a variety of F^+ sources were tested in the cyclizaiton step of ynamide. Interestingly, when selectfluor was used, Br-substituted product instead of F at 3-position was obtained. We are assuming that selectflour promote CuBr or $CuBr_2$ which generated from bromoalkyne in the ynamide synthesis process to enable Cu-catalyzed halocyclization of ynamide. As a result, it was possible to synthesize atom-economically 2-amido-3-bromobenzo[*b*]thiophene without using an external bromination reagent.In this presentation, a wide rang of substrate scopes of 2-amido-3-bromobenzo[b]thiophene and mechanistic studies will be discussed.


Previous work
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SO2R'
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2-Amido-3-bromobenzo[b]thiophene

Poster Presentation : **ORGN.P-386**

Organic Chemistry

Zoom 7 WED 17:00~17:30

Chiral Boron-based Lewis Acid Catalyzed Enantioselective Radical 1,2-Addition to Aldehydes

Jae Yeon Kim, Yea Suel Lee[1], Do Hyun Ryu[*]

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

Visible-light induced radical reaction is regarded as advantageous and attractive approach to development of efficient and selective synthetic methodology. Furthermore, this visible-light induced photoredox catalysis provides opportunities to synthesize valuable compounds easily that were previously difficult to synthesize or could be synthesized by several steps. Among those valuable compounds, 1,2-amino alcohols can be synthesized by photoredox reactions, and enantioenriched 1,2-amino alcohols are valuable in medicinal and organic synthesis due to its many synthetic utilities. Therefore, development of synthetic methods to synthesize enantioenriched 1,2-amino alcohols has been regarded as important goal. To the best our knowledge, however, catalytic asymmetric synthesis of 1,2-amino alcohol using aldehydes has been not reported. Herein, we developed boron-based Lewis acid catalyzed visible-light induced radical addition reaction to synthesize various 1,2-amino alcohol compounds with high yields (up to 99%) and high enantioselectivities (up to 98% ee).

Poster Presentation : **ORGN.P-387**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Two Bipyridine-based Organic Compounds Available As Potential Host Materials in OLEDs

Suk-Hee Moon, Youngjin Kang[1,*], Ki-Min Park[2,*]

Department of Food & Nutrition, Kyungnam College of Information & Technology, Korea
[1]*Division of Science Education, Kangwon National University, Korea*
[2]*Research Institute of Natural Science, Gyeongsang National University, Korea*

Recently the lack of examples for blue emitting materials has resulted in the resurgence in the development of blue phosphorescent materials. Henceforth, it needs an efficient molecular design incorporating bipyridine with high triplet energy and other functional unit with a suitable coordination site to metal ion through the chelation mode. The low selectivity and reactivity of pyridine ring, however, makes it very hard to introduce varied substituents into pyridine ring. In addition, it is scarce to find examples of structural characterization of bipyridine based organic compounds applicable to OLEDs performances.

In terms of OLEDs efficiency and stability, platinum and palladium complexes with tetradentate ligands are known to be very good candidates recently. The strategy of tetradentate ligand design is that the covalent C, N and O atoms are placed on a proper location of the ligand framework in order to form five- or six-membered metallacycle through C^N*C^N, N^C*C^N and C^C*N^N coordination modes while they are bound to metal(II) ion. For this purpose, 2',6'-difluoro-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine (**1**) and 2',6'-dimethoxy-6-[3-(pyridin-2-yloxy)phenyl]-2,3'-bipyridine (**2**) have been synthesized by typical cross coupling reactions and have been characterized by single-crystal X-ray diffraction. Compound **1** bearing fluorine substituents emits strong fluorescence with λ_{max} = 325 nm, while methoxy-substituted compound **2** displays red-shifted emissions with λ_{max} = 366 nm. Both compounds have high triplet energies (T_1) of 2.64 to 2.65 eV. This high triplet energy makes both compounds available as potential host materials in organic light-emitting diodes (OLEDs).

Herein, we present for the structural and photophysical characteristics depending on the different substituents of the bipyridine system in two potential dianionic tetradentate ligands, **1** and **2**.

Poster Presentation : **ORGN.P-388**

Organic Chemistry

Zoom 7 WED 17:00~17:30

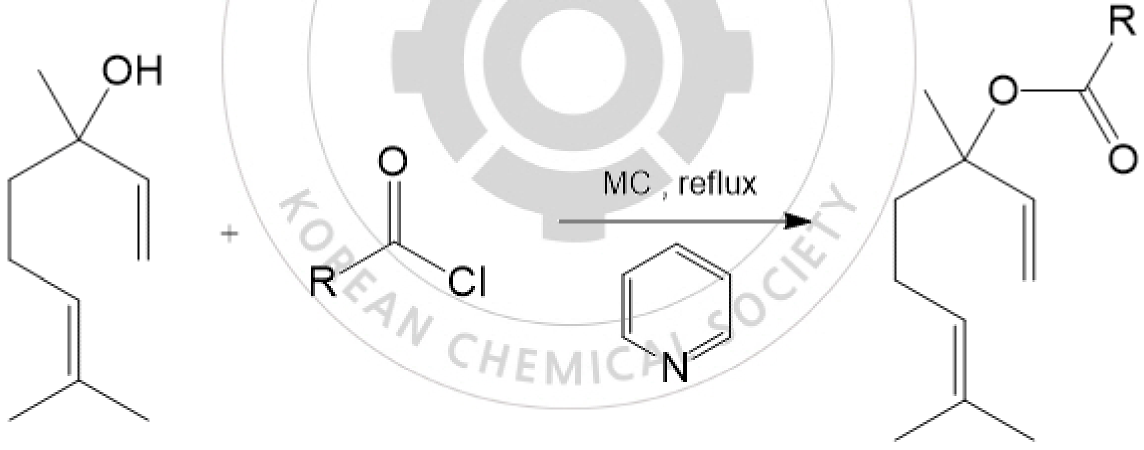
Preparation of Linalool Derivatives; Their Fragrance and Application

JiEun Lee, Chuljin Ahn[1,*]

Department of Chemitry, Changwon National University, Korea

[1]*Department of Biology and Chemistry, Changwon National University, Korea*

The linalool derivatives have been used as aroma chemicals. The known and new linalool derivatives were prepared conveniently in our lab, and were investigated their fragrance.



R : iso-butyl, Methyl, Naphthoyl, Phenyl, etc.

Poster Presentation : **ORGN.P-389**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Side-Chain Sequence Guides 2D Ordering of π-Conjugated Macrocycles on Surfaces

Soobin Kim, Henry D. Castillo[1], Zachary G. Ciesielski[1], Steven L. Tait[1,*], Dongwhan Lee[*]

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

In the surface self-assembly of rigid polyaromatics, peripheral side chains assist structural ordering by modulating the solubility and polarity at the liquid-solid interface. We now show that the “positional isomerism” of side chains around a cyclic π-skeleton can profoundly impact the energy landscape and the resulting 2D pattern, a hitherto unknown phenomenon. Macrocycles have a circular sequence. To install specific side chains at the designated positions, we have devised a modular and stepwise synthetic protocol to construct linear precursors of pre-defined sequences. An efficient intramolecular cyclization reaction of each of these molecules afforded compositionally identical yet regiochemically distinctive macrocycle isomers. STM imaging studies revealed that the sequence of the side chains around the cyclic π-skeleton profoundly impacts lateral interactions of molecules on the surface, thereby producing strikingly different 2D assembly patterns as a function of solvent polarity and surface coverage.

Poster Presentation : **ORGN.P-390**
Organic Chemistry
Zoom 7 WED 17:00~17:30

Visible-Light-Mediated C-S Bond Cleavage Reactions

Anna Lee

Department of Chemistry, Jeonbuk National University, Korea

The oxidative cleavage reaction of the C−S bond using singlet oxygen is challenging because of its uncontrollable nature. We have developed a novel method for the singlet-oxygen-mediated selective C−S bond cleavage reaction using silver(II)−ligand complexes. Visible-light-induced silver catalysis enables the controlled oxidative cleavage of benzyl thiols to afford carbonyl compounds, such as aldehydes or ketones, which are important synthetic components.

Poster Presentation : **MEDI.P-412**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Water-Soluble Organic Nanoparticles (WSONs) for Biocompatible Photodynamic Therapy (PDT) In Vitro and In Vivo

Il Yoon

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

In order to generate biocompatible PS, we successfully prepared highly water-soluble and water-stable PS from hydrophobic (not water-soluble) organic PSs using very simple and easy one-pot process by co-precipitation (solvent-exchange) method. Also highly water-soluble and water-stable PEG introduced WSONs were prepared using chlorin derivative. WSON-PEG 3400 and WSON-PEG 2000 displayed good PDT activity results against A549 and Hela cells. In vivo study using A549 tumor-bearing mice exhibited good PDT effect compared with control and drug only groups, which was confirmed by reduced tumor weight. This study will be useful in developing biocompatible PS on the basis of high water solubility as well as high water stability for PDT cancer treatment.

Poster Presentation : **MEDI.P-413**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Structure-activity Relationship Studies of Transglutaminase 2 Inhibitors

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Transglutaminase 2 (TG2) is the most extensively characterized member of the transglutaminase isozyme family, and its protein-crosslinking activity is believed to play an important role in the pathogenesis of fibro and neurodegenerative diseases. Because of the potential therapeutic relevance with these disorders, several TG2 inhibitors have been developed and most of them are glutamine-substrate mimics targeting Cys277 at the enzyme active site. Since, TG2 has a non-conserved lysine residue near Cys277, we tried to develop peptidomimetic inhibitors equipped with two electrophilic moieties, one to react with the catalytic Cys and the other to target the Lys. We also tried to develop another substrate analogs appended with a small functional group, such as hydroxyl or carbonyl, that could potentially replace a structural water molecule observed in a reported X-ray structure of a TG2-inhibitor complex. Enzyme activity assay was conducted to test the inhibitory efficiencies of the synthesized compounds, and the inhibitors with a hydroxyl group showed enhanced activities. Detailed structure-activity relationships of the synthesized compounds will be discussed.

126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **MEDI.P-414**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Fabrication of gelatin nanofiber gelma scaffolds for enhanced cell culture

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The representative extracellular matrix(ECM) hydrogel material is gelatin methacryloyl (GelMA) hydrogels. Gelma hydrogels have been used their suitable biological properties, tunable physical characteristics and essential properties similar native ECM. But gelma hydrogels have been oxygen transport limitations and cell sedimentation. gelatin nanofiber gelma scaffold will help to complement this problems.

Poster Presentation : **MEDI.P-415**

Medicinal Chemistry

Zoom 9 WED 17:30~18:00

Synthesis and evaluation of butein derivatives for in vitro and in vivo inflammatory response suppression in lymphedema

Jiman Jung, Dawn Song, Jin-Mo Ku*

Infrastructure Support Team, Gyeonggido Business & Science Accelerator, Korea

Herein, we demonstrate that butein (1) can prevent swelling in a murine lymphedema model by suppressing tumor necrosis factor α (TNF-α) production. Butein derivatives were synthesized and evaluated to identify compounds with in vitro anti-inflammatory activity. Among them, 20 μM of compounds 7j, 7m, and 14a showed 50% suppression of TNF-α production in mouse peritoneal macrophages after lipopolysaccharide stimulation. Compound 14a, exhibited the strongest potency with an in vitro IC50 of 14.6 μM and suppressed limb volume by 70% in a murine lymphedema model. The prodrug strategy enabled a six-fold increase in kinetic solubility of compound 1 and five-fold higher levels of active metabolite in the blood for compound 14a via oral administration in the pharmacokinetics study. We suggest that the compound 14a could be developed as a potential therapeutic agent targeting anti-inflammatory activity to alleviate lymphedema progression.

Poster Presentation : **MEDI.P-416**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Solid-Phase Synthesis of thiazolo[4,5-*d*] pyrimidine derivatives via Intramolecular Cyclization

<u>Su jin Lim</u>, Young Dae Gong[1,*]

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

The fused heterocycles are one of the most attractive compounds in drug discovery field due to their various biological activities. Over the years, fused pyrimidine systems including thiazolo[4,5-*d*]pyrimidine have shown various biological activities such as antitumor, antiviral, anticancer, etc. In this study, we were interested in the synthesis of thiazolo[4,5-*d*]pyrimidine derivatives via solid phase approach using traceless linker on Merrifield resin. First, the cyclization of cyanocarbonimidodithioate terminated resin with bromoacetonitrile would provide 4-amino-thiazole-5-carbonitrile intermediate. Next, imination of the intermediate with *N,N*-dimethylformamide dimethyl acetal with following treatment with various amines gives our desired thiazolo[4,5-*d*]pyrimidine core skeletons. Diversification is proceeded with a number of electrophiles like acyl chlorides, alkyl halides, sulfonyl chlorides. Interestingly, the acylation step shows the effect of protection of amine positioned in thiazolo[4,5-*d*] pyrimidine preventing oxidation of the secondary amine. After the cleavage from the resin, protection group was also removed resulting in increased yields of thiazolo[4,5-*d*]pyrimidine derivatives. Resins reacted with alkyl halides and sulfonyl chlorides underwent oxidation with mCPBA and following cleavage from the resin via amines and thiols provides diverse library of thiazolo[4,5-*d*] pyrimidine derivatives

Poster Presentation : **MEDI.P-417**

Medicinal Chemistry

Zoom 9 WED 17:30~18:00

Combination Therapy of Photodynamic Therapy Using Chlorin Derivatives and Photothermal Therapy Using Gold Nanorod

Hyeonho Song, **Il Yoon**[1,*]

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[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

Combination therapy of photodynamic treatment using new chlorin derivatives that induce apoptosis/necrosis of tumor cells by causing a reaction when exposed to light of a specific wavelength, and photothermal therapy using gold nano rod that causes damages of tumor cells by generating heat when exposed to light of a specific wavelength seems to be able to solve the problem of existing tumor treatment.

Poster Presentation : **MEDI.P-418**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

A dual inhibitor of pan-RAF and VEGFR2 for the treatment of K-RAS mutant colorectal cancer

Jaesun Jung, Soon Kil Ahn*, Goeun Lee[1], Lee JaeWoong[2], Yongbin Park[2], Ho Seok Kwon[3], Min-hyo Ki[3]

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The mitogen-activated protein kinase (MAPK) pathway plays a key role in cell survival, growth and proliferation. The cascade is regulated by extracellular signals via receptor tyrosine kinases (RTKs). In K-RAS mutant cancer, RAF-ERK pathway is upregulated. K-RAS mutations have been reported in about 40% of colorectal cancer patients. B-RAF specific inhibitors have been tested because aberrant activation of the RAF-ERK pathway is often found in K-RAS mutant cancers. However, B-RAF specific inhibitor induces RAF dimerization and paradoxical activation of C-RAF in RAS mutant cells. These facts demonstrate the discovery of pan-RAF inhibitors without causing paradoxical activation. In addition, since VEGFR2 is one of the important promoters of tumor angiogenesis in colorectal cancer, inhibition of VEGFR2 can be expected to have a synergistic effect in the treatment of colorectal cancer. By using structure-based molecular modeling, we tried to develop dual inhibitors of pan-RAF and VEGFR2. Finally, we identified a selective inhibitor, C1044 , which binds to the DFG-out inactive form of B-RAF. In addition, C1044 potentially suppressed B-RAF, C-RAF, B-RAF V600E as well as VEGFR2(IC_{50}=331nM, 257nM, 187nM and 100nM, respectively). C1044 completely suppressed the phosphorylation of MEK-ERK without paradoxical activation in K-RAS mutant cells. We investigated the effect of C1044 on the cell proliferation of K-RAS or B-RAF mutant colorectal cancer cells. To study the effects in vivo, we tested C1044 in colon cancer xenografts using mutant K-RAS. In mice with xenograft tumors, the tumor growth inhibition effect of C1044 was 96.76%(50mg/kg, oral QD).

Poster Presentation : **MEDI.P-419**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Enzymatic linking of the monomeric Phloroglucinol to high molecular oligomeric forms

Bong Ho Lee

Department of Chemical and Biological Engineering, Hanbat National University, Korea

The phlorotannins from brown seaweeds such as Ecklonia cava have diverse biological activities and being used as cosmetics, functional food ingredient, and potential medicines. Thus, the extraction and purification steps to obtain those compounds in large quantity are very important. We have shown that the phenolic monomer(phloroglucinol) can be cross-linked by chemically and enzymatically.The monomeric phloroglucinol was treated with an oxidizing agent, $K3[Fe(CN)6]$, NaOH, and SDS at room temperature, 50 ℃, 70 ℃ in few hours. It was difficult to detect any product. We did the reaction with enzymes, a vanadium-dependent either chloroperoxidase(ClPO) or bromoperoxidase (BrPO). We have changed the phloroglucinol concentration, enzyme concentration, reaction time and buffer concentration to find the optimal reaction condition. We have followed the reaction by TLC and HPLC. We were able to detect a new spot on TLC and new peaks in HPLC chromatogram. The new peaks show the products are more hydrophobic and bigger than the starting material. This results show the possibility of synthesizing oligomeric phlorotannins by oxidizing enzymes.

Poster Presentation : **MEDI.P-420**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Development of high efficient and smart anticancer drug, PDT-PTT-Chemo (PPC) triple-nanocomplex (TNC)

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There are currently various ways to treat cancer. Typical methods of treating cancer include surgery, photo-sensor, anti-cancer drugs, and radiation therapy. Among them, the method of triple therapy was conceived using optical sensitizers PDT and PTT together with anticancer drugs.Optical sensitizers are non-toxic and have the advantage of being able to selectively kill and treat cancer repeatedly. However, it is less permeable because it uses light and can cause skin toxicity by sunlight. In the case of anti-cancer drugs, they are effective in treating cancer, but they are often resistant to anti-cancer drugs, have side effects, and attack ordinary cells.Therefore, we aim to bring about selective death of cancer by converging these three methods to minimize shortcomings and maximize advantages.

Poster Presentation : **MEDI.P-421**

Medicinal Chemistry

Zoom 9 WED 17:30~18:00

A facile access to phenazine derivatives under metal-free condition

Gyeongtae Park, Giweon Yu, Seok Hun Woo*

R&D Center, ST PHARM. Co., Korea

Clofazimine has been spotlighted due to the next generation treatment of multidrug-resistant tuberculosis (MDR-TB). Due to the improved evidences found on its efficacy and tolerability, Clofazimine was upgraded to class C among the TB treatment classes designated in 2016 guidelines designated by WHO. Although some clofazimine synthesis methods have been developed, most of them include toxic metal reactions. In this study, we show a facile synthetic approach to phenazine derivative, a key intermediate of clofazimine. First of all, we use nucleophilic amination of nitrobenzene under solvent-free condition to provide excellent yield. This solvent-free reaction allows reduction of environmental pollution and improvement of purity. We then attempted reduction of nitrobenzene with sodium sulfide to provide excellent yield. This mild, metal-free reduction of nitro groups to amines not only reduces unnecessary purification step, but also gurantees high product quality. Moreover, we incorporated this new synthetic method into continuous flow technology (CFT), which has strength in safety and reproducibility of reaction. Detailed synthetic scheme and characterized will be presented in the poster.

Poster Presentation : **MEDI.P-422**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Solid-phase synthesis of thiazolo[4,5-*d*]pyrimidin-7(6*H*)-ones via iodine-based catalytic cyclization of 4-aminothiazole-5-carboxamide resin with aldehydes

Dana Kim, Young Dae Gong[1,*]

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

Solid-phase synthesis is one of the effective ways to develop diverse library of small molecule organic compounds. The heterocycles are one of the most attractive compounds in medicinal chemistry due to its various biological activities. In this respect, we were interested in the synthesis of *N*- and *S*-substituted-4-aminothiazole derivatives via solid-phase approach. First we prepared thiazole intermediate from thiourea resin with bromoacetonitrile in the presence of TEA in acetone and EtOH. The cyclized intermediate with nitrile moiety was converted to 4-aminothiazole-5-carboxamide resin by using hydrogen peroxide with potassium carbonate. Further iodine-based catalytic cyclization with diversified aldehydes gave a range number of thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one resins. Following functionalization with various electrophiles like alkyl halides, acid chlorides, and sulfonyl chlorides will provide an array of *N*-substituted-thiazolo[4,5-*d*]pyrimidin-7(6*H*)-ones. Lastly, the cleavage of the resin with amine and thiol derivatives via DIPEA in THF would generate *N*- and *S*-substituted-thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one derivatives.

Poster Presentation : **MEDI.P-423**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Synthesis of structure-based derivatives of transthyretin (TTR) to inhibit amyloid formation

Eunhee Jeon, Kunwoo Kim, Yu Jin Lee, Sungwook Choi*

Development of Drug Development and Discovery, Chungnam National University, Korea

Transthyretin (TTR) is a protein with a homotetrameric structure composed of four monomers rich in beta-sheets composed of 127 amino acids. The function of TTR is to transport the thyroid hormone thyroxine (T4) and the retinol binding protein holo through two binding sites in the blood and cerebrospinal fluid (CSF). In the brain and cerebrospinal fluid, it is mainly responsible for transporting T4, and in the blood, retinol-conjugated holo-retinol-binding protein is transported, but albumin and globulin mainly transport thyroxine in the blood, so that the binding site of TTR remains almost empty. Transthyretin (TTR), one of the 30 proteins that cause amyloidosis, is produced by misfolding and misassembly, and is known as a disease related to Senile Systemic Amyloidosis (SSA), Familial Amyloid Cardiomyopathy (FAC), and Familial Amyloid Polyneuropathy (FAP). Therefore, small molecules are used as kinetic stabilizers to prevent diseases related to TTR amyloidosis. A small molecule that binds to T4 binding site stabilize the ground state of tetrameric TTR and raise the kinetic barrier for tetramer dissociation, imposing kinetic stabilization on TTR and preventing aggregation. Currently, tafamidis (Vyndaqel), which has been approved for the treatment of FAP, and AG10, which have good activity against TTR aggregation inhibition, are known as representative small molecule compounds. Based on these structures, we have synthesized compounds that effectively suppress fibril formation, which is the cause of TTR amyloidogenesis.

Poster Presentation : **MEDI.P-424**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Synthesis and study of styryl-pyrazole derivatives that inhibit the dissociation of tetrameric TTR

Yunlan Kim, Eunhee Jeon, Yu Jin Lee[1], Kunwoo Kim[2], Sungwook Choi[2,*]

Development Of Drug Development And Discovery, Chungnam National University, Korea
[1]*Development of Drug Development And Discovery, Chungnam National University, Korea*
[2]*Development of Drug Development and Discovery, Chungnam National University, Korea*

Transthyterin (TTR) is a homotetrameric protein composed of 127-amino acid, β-sheet- rich subunits. TTR is produced by the liver and choroid plexus and it is secreted into the blood and cerebrospinal fluid(CSF). The established physiological functions of TTR are to bind and transport the thyroid hormone thyroxine (T_4) and holo-retinol binding protein in the blood and cerebrospinal fluid(CSF). However, in actual blood, albumin is present 120 times more than TTR, and globulin also has a higher affinity for thyroxine than TTR, so albumin and globulin are responsible for transporting thyroxine. Thus, most of the TTR's T_4 binding pockets in the blood remain empty. TTR is one of more than 30 nonhomologous human amyloidogenic proteins, whose misfolding and/or misassembly appears to elicit the proteotoxicity and cell degeneration, which cause the amyloidoses. In order to prevent diseases caused by such amyloid formation, styrylpyrazole based-small molecule was synthesized that inhibits the dissociation of tetramers of TTR. In fact, when thyroxine binds to the T_4 binding site, the tetrameric structure of TTR becomes much more stable. Therefore, the synthesized styrylpyrazole-based small molecule binds to the T_4 binding site and forms a covalent bond with lysine 15. Consequently, The synthesized styrylpyrazole-based small molecule further stabilizes the tetrameric TTR, helping to prevent the tetramer from dissociating into a monomer.

Poster Presentation : **MEDI.P-425**

Medicinal Chemistry

Zoom 9 WED 17:30~18:00

Discovery of a new antibiotic adjuvant agent and study on its mode of action.

So Eun Park, Hak Joong Kim[1,*]

Chemistry, Korea University, Korea

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

Antibacterial agents have been used since the 1940s and saved the lives of many people. However, due to the abusive use of these drugs led to the emergence of antibiotic-resistant bacteria. To find a new approach to overcome this problem, our laboratory attempted to discover a new antibiotic adjuvant agent, that can boost the potency of an existing, yet no longer active antibiotic drug. During our study in collaboration with Kyungpook National University Medical School, a new molecule called “CC-236096” was identified as an effective adjuvant capable of invigorating the activity of aminoglycoside antibiotics against the human pathogen *Acinetobacter baumannii*. In this poster, a preliminary result on our structure-activity relationship study as well as the initial attempt to identify its cellular target will be presented.

Poster Presentation : **MEDI.P-426**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Study of indole moiety compounds for butyrylcholinesterase inhibitors.

Jintaek Oh, Byong Wook Choi, Bong Ho Lee, Ji Hyun Hwang, Jeong Ho Park*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Indole moiety, an important heterocyclic pharmacophore in the drug-discovery. It showed biological activities such as anti-inflammatory, antioxidant, anti-tumor activity. In previous study, we synthesized the paeonol-tryptamine hybrid compounds using click reaction and evaluated their cholinesterase inhibitory activity. Tryptamine, serotonin, and melatonin have -H, -OH and -OMe functional groups at the 5th carbon position of indole, respectively. When -OMe was substituted at position 5th of the indole, the inhibitory effect on cholinergic enzyme was compared with that of the previous report having normal indole moiety. *In vitro* cholinesterase inhibitory activities were evaluated. The IC_{50} value of indole derivatives substituted with -OMe didn't have better inhibitory activity compared the previous compounds. But compounds still showed better activities (IC_{50} = 1.01 ~ 2.81μM against BuChE) than galantamine (IC_{50} = 9.4±2.5μM against BuChE).

Poster Presentation : **MEDI.P-427**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Synthesis and study of styryl-pyrazole derivatives that inhibit the dissociation of tetrameric TTR

Yunlan Kim, Eunhee Jeon, Yu Jin Lee[1], Kunwoo Kim[2], Sungwook Choi[2,*]

Development Of Drug Development And Discovery, Chungnam National University, Korea
[1]*Development of Drug Development And Discovery, Chungnam National University, Korea*
[2]*Development of Drug Development and Discovery, Chungnam National University, Korea*

Transthyterin (TTR) is a homotetrameric protein composed of 127-amino acid, β-sheet- rich subunits. TTR is produced by the liver and choroid plexus and it is secreted into the blood and cerebrospinal fluid(CSF). The established physiological functions of TTR are to bind and transport the thyroid hormone thyroxine (T_4) and holo-retinol binding protein in the blood and cerebrospinal fluid(CSF). However, in actual blood, albumin is present 120 times more than TTR, and globulin also has a higher affinity for thyroxine than TTR, so albumin and globulin are responsible for transporting thyroxine. Thus, most of the TTR's T_4 binding pockets in the blood remain empty. TTR is one of more than 30 nonhomologous human amyloidogenic proteins, whose misfolding and/or misassembly appears to elicit the proteotoxicity and cell degeneration, which cause the amyloidoses. In order to prevent diseases caused by such amyloid formation, styrylpyrazole based-small molecule was synthesized that inhibits the dissociation of tetramers of TTR. In fact, when thyroxine binds to the T_4 binding site, the tetrameric structure of TTR becomes much more stable. Therefore, the synthesized styrylpyrazole-based small molecule binds to the T_4 binding site and forms a covalent bond with lysine 15. Consequently, The synthesized styrylpyrazole-based small molecule further stabilizes the tetrameric TTR, helping to prevent the tetramer from dissociating into a monomer.

Poster Presentation : **MEDI.P-428**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Neuroprotective effect against 6-OHDA toxicity in PC12 cells resulting from the suppression of PGE_2 production by selectively blocking mPGES-1

Dohyeong Ko, Yunchan Nam, Geuntae Kim, Minji Kang, Jae Yeol Lee[1,*]

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[1]*Department of Chemistry, Kyung Hee University, Korea*

Prostaglandin E2 (PGE_2) is a bioactive lipid that elicits a wide range of biological effects associated with inflammation and is involved in various diseases including neurodegenerative diseases such as Parkinson's disease (PD) and Alzheimer's disease (AD). mPGES-1 is microsomal prostaglandin E synthase-1 that catalyses the terminal step of PGE_2 generation. Since inhibition of mPGES-1 only blocks PGE_2 production without affecting the production of PGI_2, the potential risk factors of adverse cardiovascular events, we selected mPGES-1 as a novel target for modulating neuro-inflammatory responses and neuronal function in PD. A recent report demonstrated that mPGES-1 is up-regulated in the dopaminergic neurons of the substantia nigra of postmortem brain tissue in PD patients. In particular, the fact that genetic deletion of mPGES-1 not only abolished 6-OHDA-induced PGE_2 production but also inhibited 6-OHDA-induced dopaminergic neurodegeneration both *in vitro* and *in vivo* indicate that inhibition of mPGES-1 can be a potent therapeutic strategy for the treatment of PD. In our previous study, we developed novel mPGES-1 inhibitor by extensive structure elaboration of arylsulfonyl hydrazide and arylsulfonamide derivatives from a high-throughput screening. Our representative compound **MPO-0144** shows potent mPEGS-1 inhibition activity in A549 cells, as well as neuroprotective effect in PC12 cell. Considering mPGES-1 is one of key mediators for reduction in only PGE_2, our potent mPGES-1 inhibitor **MPO-0144** may function as a promising lead compound for the treatment of Parkinson’s disease.

Poster Presentation : **MEDI.P-429**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Nitrogen and Sulfur Doped Carbon Quantum Dots as a Fluorescence Biosensor for Glutathione Detection

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[2]*Department of Chemical and Biological Engineering, Korea National University of Transportation, Korea*

Glutathione (GSH), a tripeptide and a potent anti-oxidant has been expressed in the cells and is involved in diverse biomedical reactions. However, under certain disease conditions like cancer, their levels are elevated in the cells resulting in abnormal cellular activity. Here we developed nitrogen and sulfur doped pristine carbon quantum dots (CQDs) as a novel biosensor for GSH detection. The developed CQDs demonstrated excitation independent emission, indicating that the fluorescence from CQDs is resulted from surface functional groups. The fluorescence of CQDs were selectively reduced only in the presence of GSH. The developed CQDs demonstrated a linear detection range from 0 to 600 μm and a detection limit of 15 μm. Interestingly, the developed CQDs reduced the levels of nitric oxide (NO), a potent pro-inflammatory cytokine in the LPS induced microglial cells. The results indicate a 50% reduction in the NO production when the cells were incubated with CQDs. These results demonstrate CQDs as potent biological nanomaterials for diverse biomedical applications. This work was supported by Korea National University of Transportation (2020, Yong-kyu Lee and Woo-jung Kang).

Poster Presentation : **MEDI.P-430**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Rational design of nanozymatic Ru-Te hollow nanorods for hypoxic pancreatic cancer phototherapy

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

Pancreatic cancer is a refractory carcinoma that is difficult to surgical remove and metastasize frequently. In particular, aggressive growth of pancreatic cancer induces hypoxia, oxygen depletion, which causes resistance to conviential anti-cancer drug and other types of cancer therapy. To overcome these difficulties in pancreatic cancer treatment, we retional designed ruthenium-tellurium nanorods (RuTeNRs), which has nanozymatic activity. RuTeNRs has peroxidase-superoxide dismutase (SOD) activity, produce reactive oxygen species (ROS) that cause pancreatic cancer cell apoptosis, and has catalase-like activity (CAT), convert hydrogen peroxide (H2O2) to oxygen (O2), which can relieve hypoxic condition. Also, this nanozymatc nanoparticles has excellent photo-thermal conversion efficient and photo-trigger ROS generation in the ultraviolet (UV)-visible (Vis)-near infrared (NIR) wavelength. Because of these properties, RuTeNRs wound reduce oxygen depletion and be potentialized as therapeutic candidates for hypoxic pancreatic cancer. In this study, we demonstrated that RuTeNRs-based (nanozymatic, thermo, and dynamic) combination therapy has great synergistic and therapeutic effect to hypoxic pancreatic cancer via in vitro and in vivo experiments.

Poster Presentation : **MEDI.P-431**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Synthesis of 6,7-Dihydro-5*H*-dibenz[*b,g*][1,5]oxazocin-5-one via Ullmann Coupling and Lactam Formation Reaction

Hye Ran Bae, Eunyoung Yoon[1], Jung-Nyoung Heo[2,*]

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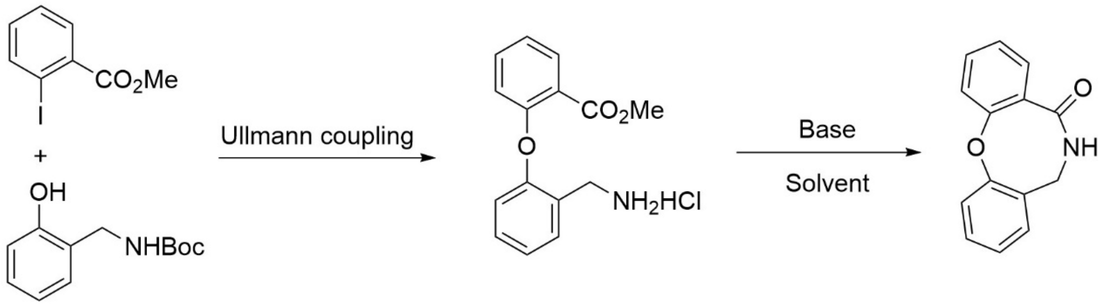
Medium-sized heterocycles (with 8 to 11 atoms) have received a lot of attention due to their unique structural features and interesting biological activities. However, it is difficult to synthesize them owing to unfavorable enthalpic and entropic factors. Herein, we present that the synthesis of dibenzoxazocine possessing the 8-membered heterocycle via ullmann coupling and lactam formation reaction.



Poster Presentation : **MEDI.P-432**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

In vivo biodistribution study of fluorescent silica nanoparticles

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Silica nanoparticles (SNPs) have proven to be promising meditator for drug delivery system. Silica nanoparticles can form various structures and morphologies, and it is easy to control their particle size and pore size as well by maintaining their structural stability. Surface modification of SNPs provides high biocompatibility. Silica nanoparticle is one of the highest nano-transmitters approved by the US FDA as GRAS (generally recognized as safe). However, although silica nanoparticles show the ideal nanocarrier characteristics for drug delivery, their delivery to specific tissues or organs in in vivo experiments need to be improved, which would eventually reduce unwanted side effects caused by SNPs. Therefore, it seems that systematic research is necessary for finding an optimal delivery system in vivo depending on the size, shape, and porosity of silica nanoparticles. In this study, we have analyzed the in vivo biodistribution of SNPs according to the particle size. The two kinds of SNPs in different sizes (25 nm and 150 nm) linked with Cy 5.5 fluorescent dye were prepared and their physical properties such as particle size, and loading efficiency were characterized. When SNPs was intravenously injected to normal SD rat, we observed that the systemic circulation last for long periods of time in case of SNP with the size below 30 nm. This preliminary study will facilitate the rational design of SNPs for their applications to drug delivery in the future.

Poster Presentation : **MEDI.P-433**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

The synthesis and biological evaluation of chalcone derivatives as a neuroprotective agent against glutamate-induced HT22 mouse hippocampal neuronal cell death

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17 chalcone analogues were synthesized from 7-methoxy-3,4-dihydronaphthalen1(2H)-one and various aromatic aldehydes under basic condition. These chalcone analogues were evaluated for the neuroprotective effects against glutamate-induced neurotoxicity. In the cell based assay, we have identified a compound C01 as neuronal cell protection agent. This compound inhibits the Ca2+ influx and cellular ROS accumulation inside the cell and the FACS analysis using annexin V and PI shows that C01 significantly reduced apoptotic or dead cell death induced by 5 mM glutamate. Further, western blot analysis indicates that glutamate induced activation of MAPKs were inhibited by compound C01 treatment. Also, the C01 increases the anti-apoptotic protein Bcl-2 and decreases pro-apoptotic protein Bax. C01 protects neuronal cells from apoptosis by preventing the translocation of AIF into nucleus. Taken together, treatment of C01 results in decreasing the neurotoxicity induced by 5 mM of glutamate. As a result, we confirm that C01 has neuroprotective effects against glutamate induced toxicity in HT22 hippocampal neuronal cells.

Poster Presentation : **MEDI.P-434**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Effects of ginsenoside Rb2 on osteogenic differentiation of C2C12 cells

Jae Wook Lee, Heesu Lee[1], Seong-Hee Ko[1,*]

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ObjectivesThe most current therapies for osteoporosis have focused on inhibiting bone resorption by osteoclasts. Although the conventional drugs have therapeutic benefits, they also have disadvantages such as breast cancer and osteonecrosis of jaw. The purpose of this study is to develop the new anabolic agents for treatment of osteoporosis that have fewer risks compared to conventional therapies. Panax Ginseng is one of the most commonly used herbal medicines. Most of the biological activities of ginseng are derived from main components, ginseng saponins (ginsenosides). To determine the effect of ginsenosides on bone formation, we examined the effect of ginsenosides Rb2(G-Rb2) on C2C12 cell proliferation and osteogenic differentiation.MethodsFor determining the effects of ginsenosides on proliferation of C2C12 cells, we did MTT assay of C2C12 cells with ginsenoside Rb1, Rb2, Rc, Rd, Rg1 and Rg3 at 0.5, 5 and 50 μM . To evaluate whether ginsenoside Rb2(G-Rb2) could promote the osteogenic differentiation of C2C12 cells, nonosteogenic precursors, mRNA expression of runt-related transcription factor-2 (Runx2) was determined. mRNA of Runx2 expression was analyzed by quantitative real time PCR. And we examined the effects of G-Rb2 on mRNA expression of estrogen receptor α and β.ResultsG- Rb1, Rb2, Rc and Rd significantly increased C2C12 cell proliferation. G-Rg3 decreased C2C12 cell proliferation at 5, 50 μM. G-Rb2 significantly increased mRNA expression of Runx2 after 24 hours culture in osteogenic media . In addition, G-Rb2 increased mRNA expression estrogen receptor α and β both. However G-Rb2 upregulated expression of estrogen receptor β to a greater extent than that of estrogen receptor α.Conclusion These results suggest that G-Rb2 may promote osteogenic differentiation of osteoblasts and may have bone protective effect through estrogen receptor upregulation.

Poster Presentation : **MEDI.P-435**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Structure guided design of novel acetylene containing 3-aminoindazoles incorporated with diarylamides as potent Breakpoint cluster region-Abelson (Bcr-Abl) kinase inhibitors endowed with anti-leukemia activity

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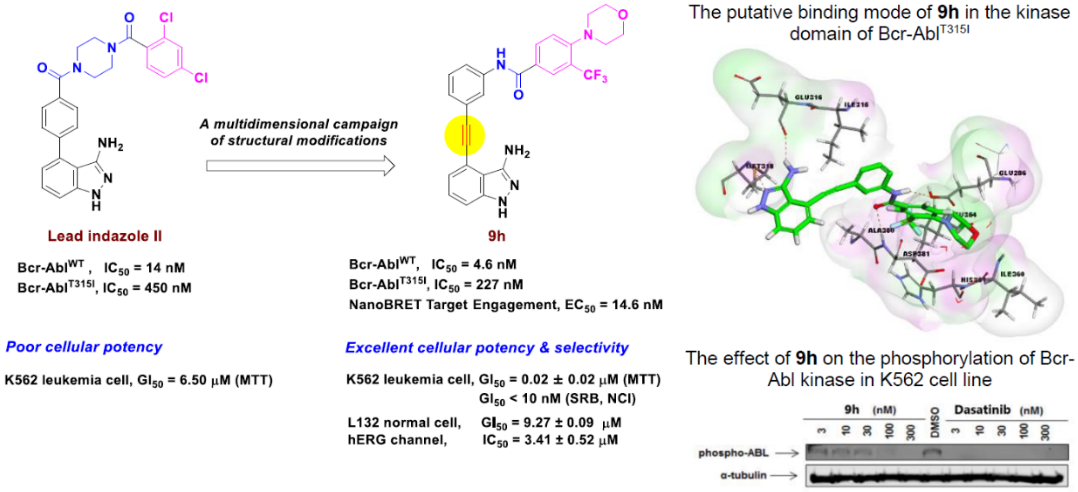
Breakpoint cluster region-Abelson (Bcr-Abl) kinase is a key driver in the pathophysiology of chronic myelogenous leukemia (CML). Broadening the chemical diversity of Bcr-Abl kinase inhibitors with novel chemical entities possessing favorable target potency and cellular efficacy is a current medical demand for CML treatment. In this respect, a new series of ethynyl bearing 3-aminoindazole based Bcr-Abl inhibitors has been designed, synthesized, and biologically evaluated. The target compounds were designed based on introducing the key structural features of ponatinib, alkyne spacer and diarylamide, into the previously reported indazole II to improve its Bcr-Abl inhibitory activity and overcome its poor cellular potency. All target compounds elicited potent activity against Bcr-AblWT with sub-micromolar IC50 values ranging 4.6–667 nM. In addition, certain derivatives exhibited promising potency over the clinically imatinib-resistant Bcr-AblT315I. Among the target molecules, compounds 9c, 9h and 10c stood as the most potent derivatives with IC50 values of 15.4 nM, 4.6 nM, and 25.8 nM, respectively, against Bcr-AblWT. Interestingly, 9h showed 2 folds and 3.6 times superior potency to the lead indazole II and 10c, respectively, against Bcr-AblT315I. Molecular docking of 9h pointed out its possibility to be a type II kinase inhibitor. Furthermore, all compounds, except 9b, showed highly potent antiproliferative activity against the Bcr-Abl positive leukemia K562 cell (MTT assay) surpassing the modest activity of lead indazole II. Moreover, the most potent members 9h and 10c exerted potent antileukemic activity against NCI leukemia panel, particularly K562 cell (SRB assay) with GI50 less than 10 nM, being superior to the FDA approved drug imatinib. Further biochemical hERG and cellular toxicity, phosphorylation assay, and NanoBRET target engagement of 9h underscored its merits as a promising candidate for CML therapy.


O
Cl
N
N
O
Cl
NH2
N
N
H
Lead indazole II
Bcr-Abl^{WT}, IC$_{50}$ = 14 nM
Bcr-Abl^{T315I}, IC$_{50}$ = 450 nM
Poor cellular potency
K562 leukemia cell, GI$_{50}$ = 6.50 μM (MTT)
A multidimensional campaign of structural modifications
H
N
O
N
O
CF3
NH2
N
N
H
9h
Bcr-Abl^{WT}, IC$_{50}$ = 4.6 nM
Bcr-Abl^{T315I}, IC$_{50}$ = 227 nM
NanoBRET Target Engagement, EC$_{50}$ = 14.6 nM
Excellent cellular potency & selectivity
K562 leukemia cell, GI$_{50}$ = 0.02 ± 0.02 μM (MTT)
GI$_{50}$ < 10 nM (SRB, NCI)
L132 normal cell, GI$_{50}$ = 9.27 ± 0.09 μM
hERG channel, IC$_{50}$ = 3.41 ± 0.52 μM
The putative binding mode of 9h in the kinase domain of Bcr-Abl^{T315I}
GLU316
ILE316
MET318
GLU286
ALA380
ASP381
HIS361
ILE360
The effect of 9h on the phosphorylation of Bcr-Abl kinase in K562 cell line
9h (nM)
3
10
30
100
300
DMSO
Dasatinib (nM)
3
10
30
100
300
phospho-ABL
α-tubulin

Poster Presentation : **MEDI.P-436**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Virtual Screening for Selective drug Discovery

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New drug design research using computer studies the relationship between 2D/3D quantitative structure and activity of target protein, derives pharmacophore model, which is essential for pharmacological activity that substrate should have, proceed screening to select the optimal inhibitor. Computer-aided drug design studies are divided into structure- and ligand-based drug design. Structure-based drug design is to design a pharmacophore model for amino acid residues in active sites based on the 3D structure of the target protein under study. Ligand-based drug design predicts the activity of a new candidate compound by designing a pharmacophore model and a quantitative structure-activity relationship model using information of compounds known to be active against a target protein. In this study, selective inhibitors were designed using both methods. Ligand-based pharmacophore model consisting of ring aromatic, positive ionizable, negative ionizable, and hydrogen bonding receptors were generated from known active inhibitors. In addition, by analyzed the binding modes of known target proteins and ligands, we generated a structure-based pharmacophore model with the addition of hydrogen bonding donors. To increase bioavailability from a total of 1,890,602 commercial drug candidates databases, Lipinski's rule of five and ADMET analysis were used to filter 178,161 chemical compounds for virtual screening. After that, 20 selective inhibitors were finally selected through the process of selecting compounds with a fit value of 3.52 or higher and eliminating duplication.

Poster Presentation : **MEDI.P-437**
Medicinal Chemistry
Zoom 9 WED 17:30~18:00

Resistance to tyrosine kinase inhibitors originated from the altered EGFR mutant-specific interactome

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Non-small cell lung cancer (NSCLC) is the major class of lung cancers and constitutes for more than 80% of patients diagnosed in the metastatic stage. NSCLC is believed to be progressed with genomic alterations such as mutations on EGFR or KRAS and amplifications of HER2 or MET. Thus, targeting of activating mutations within epidermal growth factor receptor (EGFR) using tyrosine kinase inhibitors (TKIs) has been the standard of care for patients with NSCLC. Although progression-free survival was initially appeared to be improved, overall mortality at the end remains dismal mainly due to the resistance to TKIs. Studies have been carried out to understand causes of acquired EGFR-TKIs resistance. Nevertheless, how the resistance is acquired during the course of TKI treatment remains to be understood. To resolve this challenging question on the origin of the TKI resistance, we hypothesize that TKI may alter EGFR interactome which leads to acquired resistance through de novo mutation of EGFR. To test our hypothesis, we will characterize mass spectrometry-based EGFR interactomes upon TKI treatment on lung cancer cell lines harboring acquired TKI resistance mutations such as EGFR T790M mutation, c-MET amplification and HER2 amplification. This result would deepen our understanding about acquired EGFR-TKIs resistance mechanisms and may reveal targets for preventing TKIs resistance development. *Keywords: NSCLC, EGFR mutations, TKI resistance, EGFR interactomes.

Poster Presentation : **MAT.P-438**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Evaluation of raw and calcined eggshell for removal of Cd2+ from aqueous solution

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The potential use of egg shell and calcined egg shell as adsorbent was evaluated and compared to remove Cd2+ from aqueous solution. The samples were characterized using Thermogravimetry and Differential Thermal Analysis (TG/DTA), Scanning Electron Microscope (SEM), X-ray Diffractometer (XRD), Energy Dispersive X-ray Spectrometer (EDX) and BET Surface Analyzer. The batch-type adsorption experiment was conducted by varying diverse variables such as contact time, pH, initial Cd2+ concentrations and adsorbent dosage. The results showed that, under the initial Cd2+ concentrations ranged from 25 to 200 mg g-1, the removal efficiencies of Cd2+ by egg shell powder (ESP) were decreased steadily from 96.72 % to 22.89 % with increase in the initial Cd2+ concentration at 2.5 g of dosage and 8 h of contact time. However, on the contrary to this, calcined egg shell powder (CESP) showed removal efficiencies above 99% regardless of initial Cd2+ concentration. The difference in the adsorption behavior of Cd2+ may be explained due to the different pH values of ESP and CESP in solution. Cd2+ seems to be efficiently removed from aqueous solution by using the CESP with a basicity nature of around pH 12. It was also observed that an optimum dosage of ESP and CESP for nearly complete removal of Cd2+ from aqueous solution is approximately 5.0 g and 1.0 g, respectively. Consequently, Cd2+ is more favorably adsorbed on CESP than ESP in the studied conditions. Adsorption data were applied by the pseudo-first-order and pseudo-second-order kinetics models and Freundlich and Langmuir isotherm models, respectively. With regard to adsorption kinetics tests, the pseudo-second-order kinetics was more suitable for ESP and CESP. The adsorption pattern of Cd2+ by ESP was better fitted to Langmuir isotherm model. However, by contrast with ESP, CESP was described by Freundlich isotherm model well.

Poster Presentation : **MAT.P-439**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Evaluation of natural and calcined eggshell as adsorbent for phosphorous removal from water

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Natural and calcined eggshell as adsorbent alternatives were evaluated for the removal of phosphorous from water. Calcined eggshell was obtained after treating the natural eggshell at 900oC in electric furnace for 2 h. The examination on their characteristics was carried out with Thermogravimetry and Differential Thermal Analysis (TG/DTA), Scanning Electron Microscope (SEM), X-ray Diffractometer (XRD) and Energy Dispersive X-ray Spectrometer (EDX). The working solution containing phosphorous was prepared by dissolving KH2PO4 with distilled water. The batch adsorption experiment was conducted by changing various variables such as initial phosphorous concentration, dosage of natural and calcined eggshell, contact time and pH. It turned out that natural eggshell was unable to remove phosphorous from water, whereas a considerable amount of phosphorous by calcined eggshell was removed in initial contact time (0.25 h). The removal efficiencies were found to be 99.5 and 99.28 % at experimental conditions of 5 mg g-1 of initial phosphorous concentration and a 1.0 g of calcined eggshell dosage, respectively. The removal efficiencies of phosphorous by calcined eggshell were dependent on the above-mentioned variables. The difference in the removal behavior of phosphorous by natural and calcined eggshell may be explained due to the different pH values and Ca2+ concentration in solution. The research results suggested that phosphorous removal mechanism by natural eggshell is caused by adsorption of phosphate (as phosphorous source) onto the surface of natural eggshell, however, on the contrary to this, the phosphorous removal on calcined eggshell is arisen from the binding of phosphosphate and calcium resulting in precipitation of calcium phosphate. Experimental data were applied by the pseudo-first-order and pseudo-second-order kinetics models and Freundlich and Langmuir isotherm models, respectively. The pseudo-second-order kinetics model and Langmuir isotherm model were more suitable for calcined eggshell owing to the higher correlation coefficient R2. In conclusion, the result showed that calcined eggshell could become a favorable adsorbent material for removing phosphorous from water.

Poster Presentation : **MAT.P-440**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Study on Adsorption of PO43--P in Water using Activated Clay

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In this study, activated clay treated with H2SO4 (20% by weight) and heat at 90oC for 8 h for acid white soil was used as an adsorbent for the removal of PO43-P in water. Prior to the adsorption experiment, the characteristics of activated clay was examined by X-ray Fluorescence Spectrometry (XRF) and BET surface area analyser. The adsorption of PO43--P on activated clay was steeply increased within 0.25 h and reached equilibrium at 4 h. At 5 mg/L of low PO43--P concentration, roughly 98% of adsorption efficiency was accomplished by activated clay. The adsorption data of PO43--P were introduced to the adsorption isotherm and kinetic models. It was seen that both Freundlich and Langmuir isotherms were applied well to describe the adsorption behavior of PO43--P on activated clay. For adsorption PO43--P on activated clay, the Freundlich and Langmuir isotherm coefficients, KF and Q, were found to be 8.3 and 20.0 mg/g, respectively. The pseudo-second-order kinetics model was more suitable for adsorption of PO43--P in water/activated clay system owing to the higher correlation coefficient R2 and the more proximity value of the experimental value qe,exp and the calculated value qe,cal than the pseudo-first-order kinetics model. The results of study indicate that activated clay could be used as an efficient adsorbent for the removal of PO43-P from water.

Poster Presentation : **MAT.P-441**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Polypyrrole Composites for Cell Scaffolds

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An elctroactive polypyrrole composite is prepared onto the surface of polypyrrole films by electrochemically polymerizing 1-(2-carboxyethyl)pyrrole monomer that was synthesized from 1-(2-cyanoethyl)pyrrole. FTIR is used to demonstrate the successful incorporation of carboxylic acid (-COOH) groups onto the polypyrrole composite and a four-point probe analysis is used to verify electrical conductivity in the semiconductor range. Carboxylic acid functionality of the composite is then tailored by chemically conjugating a cell-adhesive Arg-Gly-Asp (RGD)-containing peptide, GRGDSP, onto the surface of composite. Further studies are currently underway to evaluate cellular activity of the composite to adhere to the surface and spread. Here, the preparation and properties of bioactive scaffold based on RGD-functionalized polypyrrole composites are presented and discussed. This was supported by Korea National University of Transportation in 2020.

126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **MAT.P-442**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Janus solar oil evaporation systems for cleanup and collection of BTX

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[1]*Chemical and Biological Engineering, Hanbat National University, Korea*

Oily wastewater has become one of the most severe global challenges, resulting in serious long-term effects on the ecosystem as well as on public health. Superhydrophobic or superhydrophilic materials have been developed for efficient oil/water separation. The purpose of most oil/water separation is cleanup of spilled oils. A little attention has been focused on collection of spilled oil using oil/water separation techniques. Furthermore, collection techniques of Benzene, Toluene, and Xylene (BTX) that are expensive and highly toxic are very important for environmental and economic reasons. To the best of our knowledge, however, it has not yet been reported. We have developed a novel unmanned evaporation and collection system using solar oil evaporation.

Poster Presentation : **MAT.P-443**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Unmanned solar oil evaporators for fast cleanup of hazardous noxious substance (HNS)

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[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Global water resources have been polluted owing to increasingly frequent oil spill accidents and industrial oily wastewater. Thus, oil/water separation has recently become an important issue in scientific research and practical applications. Furthermore, spill accidents of Benzene, Toluene and Xylene known as expensive and useful solvents have frequently occurred. However, BTX can damage the liver, kidney and central nervous system due to their toxicity and carcinogenicity. Thus, the development of unmanned system for cleanup and collection of BTX is highly necessary. We report here photothermal conversion-based solar oil evaporation system for cleanup of BTX.

Poster Presentation : **MAT.P-444**

Materials Chemistry

Zoom 8 WED 16:30~17:00

Eco-friendly series and parallel air filters for removal of particulate matters and volatile organic compounds

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Air pollution by particulate matter (PM) has become one of the most severe global challenges in the 21st century. PMs are a complex entity composed of sulfates, nitrates, ammonium, soot, sea salt, silicates, trace metals, carbonaceous material, and water. Prolonged exposure to PMs can lead to respiratory disease, cardiovascular disease, and even cancer. Therefore, there is an increasing demand for developing high performance air filters with low pressure drop. The development of abovementioned air filter is one of important challenging tasks because there is trade-off between filtration efficiency and pressure drop. We report eco-friendly novel air filtration system with high filtration efficiency and low pressure drop.

Poster Presentation : **MAT.P-445**
Materials Chemistry
Zoom 8 WED 16:30~17:00

In-situ X-ray absorption spectroscopy analysis of hollow RuO2/TiO2 composites for application to advanced anode material of LIBs

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TiO2 has been studied for a long time as an electrode material in lithium ion batteries (LIB) because it has a long life, low cost, and little impact on the environment. Low electrical conductivity of TiO2 has been an inherent drawback when it is applied to LIBs. In this study, RuO2 with a high electrical conductivity was used as an additive to compensate for the poor conductivity of TiO2. In addition, a hollow spherical nanocomposite was manufactured in order to buffer the volume expansion that occurs during charge and discharge, which is a chronic problem of transition metal oxides. As a result, the high energy density and good conductivity of RuO2 can compensate for the low conductivity of TiO2. In-situ X-ray absorption spectroscopy analysis was performed to confirm the charge compensation mechanism and Ru atom environment that occur during the charge/discharge cycle of RuO2/TiO2 hollow spheres used as lithium-ion battery anode materials. During the charge-discharge cycle, XAS data collected at Ru edges about every 10 minutes showed details of charge/discharge mechanism. The XANES and EXAFS spectra provided information on the Ru atomic environment, such as oxidation state and structural changes during cycling and the distance between adjacent atoms.

Poster Presentation : **MAT.P-446**
Materials Chemistry
Zoom 8 WED 16:30~17:00

An anatomical comparison of human terminal hairs: Microscopic observation and Properties

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[1]*Institute of Biological Interfaces, Sogang University, Korea*

Human has various type of hairs, which can be roughly classified into scalp hair and androgenic hair. All the hairs mainly consist of keratin protein and share a common structure of cuticle, cortex, and medulla. Although scalp hair has been studied a lot in the field of cosmetics, the androgenic hairs are still lacking in research. Including their internal structure and characteristics against the external environment. In this study, we observed the surface and internal structure of various hair with microscopic devices, such as LV-EM and FT-IR. Also, the characteristics of various hair depending on the different external environments, such as high/low pH, sweat, and urine are studied.

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Poster Presentation : **MAT.P-447**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Fabrication of Flexible Pressure Sensor with 3D Printing Method

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Elastic nanocomposite piezoresistive pressure sensors have recently received considerable attention in many areas due to their broad applications, such as robotics, wearable flexible electronics, electronic skin (E-skin) and medical devices. In order to meet the requirements to a specific application,, those piezoresistive pressure sensors must be further advanced in terms of sensitivity, manufacturing easiness, flexibilities or stability. We fabricated piezo-electric sensors and working devices, having various internal 3D structures and shapes using a home-made 3D printable CNT/PDMS ink. Although the ink used here was the same formulatio with the same electrical characteristics, their sensitivities upon different mechanical stimulus were widely varied. We would like to present variously designed pressure sensors and transducers, which were implemented with various types of 3D designs and shapes, and show how their sensitivities and mechanical properties could be controlled.

Poster Presentation : **MAT.P-448**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Synthesis and Characterization of Novel Two-dimensional Quaternary Bismuth Sulfide of $KAgBi_2S_4$

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In an effort to search for novel quaternary bismuth sulfide compounds, we have explored K/Ag/Bi/S system and encountered novel quaternary bismuth sulfide compound, $KAgBi_2S_4$ using K_2S_x molten salt at intermediate temperature. The black hexagonal crystals of $KAgBi_2S_4$ are obtained at 300℃ and crystallized in the space group P63/mmc (no.194) with a=4.0216(3)Å, c=30.066(3)Å, γ=120°, Final R/wR_2=4.37/13.15%. The structure of $KAgBi_2S_4$ is composed of negatively charged Bi_2S_3-type layers separated by charge balancing K^+ ions which are loosely packed in the interlayer spaces. Substitution of Ag atom for Bi atoms requires another cation to balance charge and the resulting Bi_2S_3-type $[AgBi_2S_4]^-$ fat layers with heavily disordered K^+ ions. Diffuse reflectance measurement revealed the semiconducting behavior with band gap value of 0.96eV.

Poster Presentation : **MAT.P-449**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Humidified air treated C_3N_4 nanoplatelets and their in vivo fluorescence imaging performance without labeling

Sungjin Park[*], **Dawoon Jang**

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In this work, we develop a route to produce a novel bioimaging probe framework. A C_3N_4 material (UCN-H) is produced by thermal condensation of urea under humidified air treatment. Chemical characterizations reveal that the UCN-H contains C_3N_4 network with smaller grain sizes and more amine-based functionalities at the edges than UCN, which is separately produced without the humidified air treatment. Highly stable aqueous dispersions including fluorescent C_3N_4 nanoplatelets are generated by sonication of the UCN-H powder. The photoluminescence (PL), time resolved-PL, and 2D excitation-emission spectra of the dispersions show that the UCN-H has less-intra bandgap traps and longer PL lifetime than UCN. In confocal microscopic study using the nanoplatelets, clear fluorescent cell-images are obtained without any cytosolic aggregation. In in vivo imaging studies with MDA-MB-231 tumor- bearing mice models, persistently strong fluorescence signals are successfully observed on tumor lesions without any interference of auto-fluorescence from live tissues after their accumulation by passive tumor targeting. Ex vivo biodistribution and histology results are well-matched with in vivo fluorescence imaging results.

Poster Presentation : **MAT.P-450**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Electrocatalysis for the oxygen evolution reaction: synthesis of NiO/N-doped carbon hybrid and its electrocatalytic activity

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Oxygen evolution reaction (OER) is one of the most important steps at an anode in electrochemical water splitting process and needs excellent electrocatalysts to improve overpotentials. The price of precious metal has interfered practical application, even though precious metal-based materials, such as RuO2, IrO2 and their hybrid with other components showed outstanding activity as OER electrocatalysts. accordingly, earth-abundant metal components including Fe, Co, and Ni have been investigated as alternatives. In our work, the hybridization of Ni-containing species with conductive carbon-based materials was used to prevent aggregation of active species and improve electrochemical catalytic performance. A new hybrid material composed of NiO nanoparticles and N-doped carbon materials was prepared. The NiO particles with a narrow size distribution were well dispersed on the surface of carbon-based materials. The hybrid showed improved electrocatalytic performance for OER than single components of NiO and N-doped carbon materials.

Poster Presentation : **MAT.P-451**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Formation of Cellular Multi component Extracellular Matrix

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Extracellular matrix is a connective fiber network supporting cells living to its surrounding environment. Particularly, In basal region of skin tissue, a multi-component extracellular matrix, mainly composed of fibronectin (FN), laminin (LAM) and collagen (COL) are formed in forms of fibers. That provide the physical and mechanical stability, and intercellular communication necessary for tissue morphogenesis and homeostasis. Here, we harnessed the fibrillogenesis to architecture the multi-component extracellular matrix. We simultaneously and subsequentially manipulated the ECM components network by depositing various ECM molecules (FN, LAM and COL) to drive cellular ECM synthesis. We found that cell-derived FN network could be grown from all of the ECM components, pre-deposited on a surface. Although the FN and COL have been known to induce FN fibrillogenesis reciprocally, however, interestingly, we also found that FN fibrillogenesis could induced by LAM. The unfolded and extended FN fibril formatiion were confirmed by fluorescence resonance energy transfer (FRET) assay. We believe that this study could provide a controllable multi-component ECM network fabrication as a novel platform for cell-mimicking ECMs in tissue engineering.Keywords: extracellular matrix, fibronectin, laminin, collagen, FRET

Poster Presentation : **MAT.P-452**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Label-Free Detection of Biomarker with Ultra-high Sensitivity using an Electrolyte-gate Thin-Film Transistors (TFTs) structure

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Early diagnosis for some disease such a Alzheimer's disease, Parkinson's disease is so important because these diseases are difficult to treat after the onset. For early diagnosis of disease, it is required that technique for detecting trace amount biomarkers. However, research on this has not been actively studied. In this study, we presents a new strategy for highly sensitive protein detection at femtomolar levels without any labelling has been demonstrated by using an electrolyte-gate Thin-Film Transistors (TFTs). Thin-Film Transistors have high sensitivity, low cost, flexibility, and it can be applied to mass production based on easy fabrication. We had demonstrated effective electrode protecting for using electrolyte-gate via thiol-ene click reaction. this device is fabricated via UV curing. This device fabrication with 1,10-decanedithiol, Vinyl-POSS, Octadecanethiol And it function well in repeated experiments. This device assembled cognitive function groups using APTES, Glutaraldehyde, and Aptamer to detect biomarker and a limit of detection (LOD) of 1 fM were achieved by using this device.

Poster Presentation : **MAT.P-453**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Exploration of Substituents Engineered Deep-Red to NIR Emitting Phosphorescent Complexes for Solution-Processable Organic Light-Emitting Diodes

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NIR emitting chromophores have tried to solve critical challenges such as the vulnerability of the small emissive band gap towards several non-radiative decay pathways including overlap of ground and excited state vibrational energies and high frequency oscillators. In order to investigate the effects of electron withdrawing and donating substituents which are anchored on the quinoline moiety of (benzo[b]thiophen-2-yl) quinoline cyclometalating ligands, we synthesized deep-red to NIR emitting iridium(III) complexes. In perspective of photophysical studies, we executed experiments in solution, doped polymer film, powder and at 77 K to examine the effects of substitution on the excited state characteristics. Single crystal X-ray structures authenticated the exact coordination geometry and intermolecular interactions and theoretical parameters were calculated by DFT and TD-DFT calculation. Measurement in doped polymer films, the -CH3 substituted (Ir1), unsubstituted (Ir2) and -CF3 substituted complex (Ir4) were represented high phosphorescence quantum efficiency. We fabricated unoptimized deep-red to NIR OLED device by solution processing. The maximum EQE values were 2.05% (Ir1) and 2.11% (Ir2).

Poster Presentation : **MAT.P-454**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Thermoelectric performance of hole doped-polycrystalline Sn$_{1-x}$Fe$_x$Se

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Thermoelectric (TE) materials can contribute to solving energy problems that because it can directly convert waste heat into electric energy. SnSe single crystals have shown exceptionally high thermoelectric figure of merit (ZT) of ~2.6 at 923K along the b-axis due to a highly anharmonic bonding. However, it takes a lot of time and cost to obtain high-quality single crystal samples. Therefore, mass production of this material is unsuitable. Although the polycrystalline SnSe samples have strengths in device applications because they have machinability and scalability, they have much poorer than single crystal samples. Therefore, achieving TE properties of polycrystalline SnSe samples similar to or higher than single crystal samples are one of the most important studies. However, it is quite difficult to make a high ZT polycrystalline SnSe material because of both low dopability and solubility limit with other elements.In this presentation, we investigated the doping effect of Fe for polycrystalline SnSe systems to improve their TE properties. At the optimal level, Fe doped SnSe increases power factor due to the increase electroconductivity While maintaining the Seebeck coefficient. As a result, the best performing system achieves a high ZT larger unity at 800K.

Poster Presentation : **MAT.P-455**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Block copolymer templated mesoporous Mg-Al mixed metal oxide for effective Congo red removal

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Effective adsorption of Congo red (CR) dye from an aqueous solution with maximum adsorption efficacy was achieved by mesoporous Mg-Al mixed metal oxide (MMO) prepared with pluronic P-123 template. Two kinds of MMOs were obtained by calcining of layered double hydroxides which were synthesized utilizing P123 template under respective solvents, ethanol and water; each MMO was designated MMO-E and MMO-W. According to the electronic microscopies, MMO-E had sand-rose morphology with random interparticle pore whereas MMO-W had an assembly of small particles with relatively uniform interparticle cavities. Adsorption kinetics of CR on MMO-E and MMO-W was well-fitted to the pseudo-second-order kinetics, suggesting strong adsorbent-adsorbate interaction. Adsorption isotherms were well described by the Langmuir model for MMO-E and Freundlich model for MMO-W, respectively, indicating effective multilayer adsorption on MMO-W. Due to the different adsorption mechanisms, the maximum adsorption of CR was different with respect to MMO type, 1517 mg/g for MMO-E and 3470 mg/g for MMO-W. It was concluded that different particle morphology and interparticle arrangement in MMO governed the dye removal efficacy.

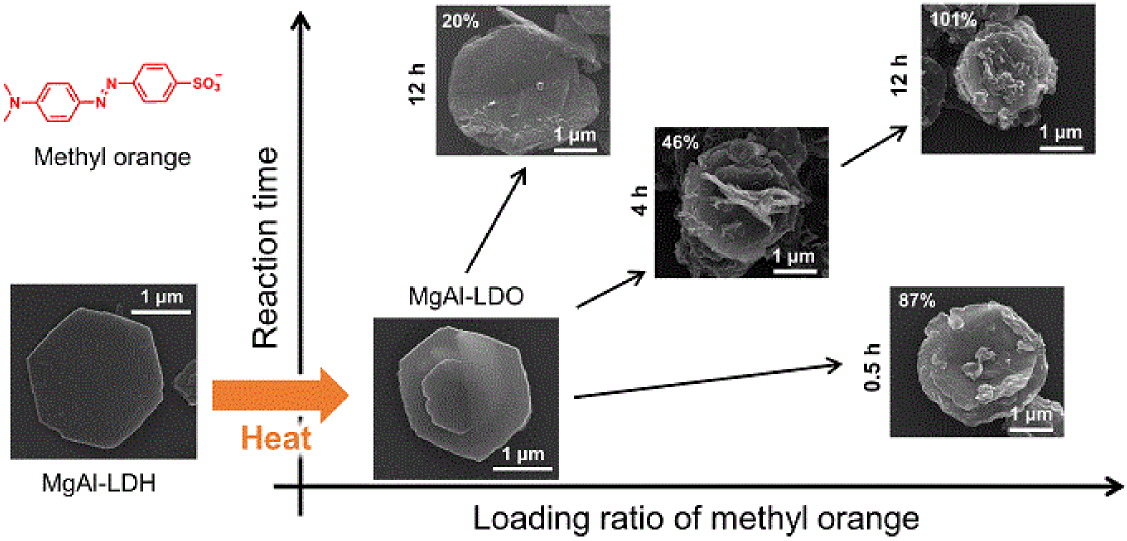
Poster Presentation : **MAT.P-456**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Controllable surface roughness of reconstructed LDH by methyl orange intercalation

Tetsuo Yamaguchi, Jae-Min Oh*

Department of Energy and Materials Engineering, Dongguk university, Korea

Control of surface roughness expects development of energy saving and sustainable economic systems by inducing beneficial phenomena like superhydrophobicity, antireflection property. Layered double hydroxides (LDHs) are known as an environmental-friendly and biologically compatible materials which consisted of metal hydroxide sheet and interlayer anion. Calcination of LDHs induced dehydration to give layered double oxides (LDOs) and the LDOs returned to the LDHs by rehydration with partial roughening of the particle surface [1] although this phenomenon is not fully comprehended. In this presentation, we will report the control of the surface roughness of MgAl-LDH by concentration and reaction time in methyl orange aqueous solutions. The relatively large molecule, methyl orange, was found to roughen surface of reconstructed LDH through hindering ordered layer stacking. Furthermore, higher concentration and longer reaction time gave the rougher surface of the reconstructed LDH as shown in Fig. 1. Reference: [1]B.K. Kim, G.H. Gwak, T. Okada, J.M. Oh, J. Solid State Chem. 263 (2018) 60–64.


Methyl orange
SO_3^-
MgAl-LDH
1 μm
Heat
Reaction time
MgAl-LDO
1 μm
12 h
20%
1 μm
4 h
46%
1 μm
12 h
101%
1 μm
0.5 h
87%
1 μm
Loading ratio of methyl orange

Poster Presentation : **MAT.P-457**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Synthesis of core-shell structure silica sphere for a thermal energy storage medium using various paraffin wax as phase change materials

Hanjun Mun, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

As a solution to the urban heat island phenomenon, instead of creating a green area,The method applied to the roof or ceiling of a building is drawing attention. Paraffin wax is an excellent phase change material and has the advantage of absorbing and releasing heat in various temperature ranges. Paraffin-water emulsion encapsulation is required for application to building materials. In this study, paraffin wax was encapsulated with SiO_2 through the sol-gel method to synthesize a silica sphere having a size of about 200 nm to 600 nm. Thermal storage efficiency according to the type of paraffin wax was compared through DSC. The morphology of the synthesized material was observed using TEM and SEM. The correlation between paraffin wax and heat storage efficiency was investigated.

Poster Presentation : **MAT.P-458**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Synthesis of porous silica network with controllable pore size from slag

Gyuhwan Hwang, Namho Kim, Jae-Min Oh*

energy and materials engineering, Dongguk University, Korea

Porous silica with controllable pore size from micropore to macropore was successfully obtained from slag. Lumps of slag produced during alloy process was determined to have 21.6 % of CaO, 33.9 % of SiO2, 17.0 % of MnO and 14.0 % of Al2O3 by X-ray fluorescence spectroscopy. In order to dissolve metal species in controlled manner and to obtain porous silica, slag lumps were crushed and classified by the piece size, above 38 μm, between 75 μm and below 400 μm. Then it was then treated with HCl with respective concentration of 3 and 6 mol/L and treatment time of 4 and 24 h. Final product was filtered, washed with deionized water and dried under vacuum. The nitrogen adsorption-desorption isotherms showed that acid treatment to produce microporous structure with large starting size (> 75 μm) and mesoporous structure with small size (< 38 μm). The specific surface area generally showed increasing value according to high acid concentration, small starting size and long reaction time; the specific surface area became decrease when the concentration at 6 M HCl, starting size between 38 and 75 μm, and 24h reaction time. The largest specific surface area 632.8 m2/g, pore volume 0.31 cm3/g with microporous silica was obtained when 3 mol/L hydrochloric acid was treated to 75 μm slag for 24h.

Poster Presentation : **MAT.P-459**

Materials Chemistry

Zoom 8 WED 16:30~17:00

Effect of halogen and sulfur substitution in Li5.5PS4.5X1.5 (X= Cl, Br)

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Department of printed electronics engineering, Suncheon National University, Korea

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As the Energy storage system (ESS) and electric vehicles (EVs) market grows, large-scale lithium-ion batteries (LIBs) are attracting attention. However, Liquid-based batteries have limitations in that have fire stability and lower energy density that all-solid-state-batteries (ASSBs). In order to overcome this limitation, a lot of effort has been conducted for the development of a Li-ASSBs. A number of studies such as halogen and sulfur substitution(Li6PS1-ySey5X, x= Cl, Br, I, y=0~1), aluminum doping(Li6-3xAlxPS5Cl), Li-rich argyrodite, etc. have been conducted. and improvement of ionic conductivity has also been reported(~6mS/cm in Li5.7PS4.7Cl1.3). however, it still has drawback of having insufficient conductivity compared with the other Li-conductors.In this work, we describe the change o ionic conductivity with the replacement of sulfide and chloride anions by selenide and bromide. Various argyrodite, Li5.5PS4.5-ySeyCl1.5-xBrx (x, y = 0~1.5) are synthesized in a sealed quartz and the electrochemical properties are characterized.

Poster Presentation : **MAT.P-460**
Materials Chemistry
Zoom 8 WED 16:30~17:00

Layered double hydroxide and oxide with controlled porous structure prepared with natural template

Jiwon Park, Sang-Yong Jung, Jae-Min Oh*

Material and of Energy engineering, Dongguk University, Korea

Layered double hydroxide (LDH) and its calcined form, layered double oxide (LDO), with porous structure and high specific surface area were prepared with natural templates. First of all, LDH@A was prepared in the protein (albumin from chicken egg white, size ~6.5 nm) solution and calcined at 500□C to obtain LDO@A. The LDO was reconstructed under albumin solution to produce LDH@A-2, which was again calcined (LDO@A-2). The specific surface area was 65.2, 176.6, 107.8, 224.3 m2/g for LDH@A, LDO@A, LDH@A-2 and LDO@A-2, respectively, showing fairly increased value compared with previous reports. As we found that protein act as a porogenic template, unpurified protein, egg-white was directly utilized to produce porous LDH and LDO. Coprecipitation of metal salt solution was carried out under egg white (EW) foam, which was homogeneously prepared with a household hand blender. The specific surface area of as-prepared LDH@EW was fairly high showing 168.98 m2/g and the pore was determined mesoporous. According to the scanning electron microscopy, the LDH@EW had sandrose of which interparticle space develop mesopores. After calcination, the LDO@EW was determined to have preserved specific surface area of 176.62 m2/g of which mesopore was narrowly distributed at 15.9 nm showing controlled porous structure.

Poster Presentation : **MAT.P-461**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Synthesis of *1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane*(FD3) derived fluro siloxane resin compound added *Trifluoropropyltrimethoxysilane*(TFPTMS)

Ji Myeong Lee, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

Resin type siloxane has been used in various researches as coating materials. Among them, flourine functional group, known as having hydrophobic and oleophobic properties on surface, is very attractive as a coating material. In the past, various types like oil, resin, powder etc. have been sythesized using multi-functional alkoxide silane. In this research, fluoro siloxane resin compound(FSR) was synthesized using D type fluoro alkoxide silane mainly and T type fluoro alkoxide silane for more functional groups.FSR was sythesized using *1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl)cyclotrisiloxane*(FD$_3$) as a D type precursor and *Trifluoropropyltrimethoxysilane*(TFPTMS) as a T type precursor. The synthesis has been progressed controlling the concentration of hydrolysis agent and the reaction temperature.For analysis, Nuclear Magnetic Resonance(^{29}Si NMR) and Fourier Transform Infrared spectoscopy(FT-IR) were used for confirming the siloxane group(Si-O-Si) and silanol group(Si-OH). Gel Permeation Chromatography(GPC) was used to confirm the molecular weight of intermediate progress and final acquired FSR. X Ray Diffraction(XRD) analysis was used to reveal its structure.

Poster Presentation : **MAT.P-462**
Materials Chemistry
Zoom 8 WED 17:00~17:30

The Synthesis and Characterization of Highly Water Soluble Triphenylmethine Acid Dyes for Digital Textile Printing

Seong Hyun Jang, Lee Geonho, Sang Yoon Lee[1], Jun Choi[*]

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Digital Textile Printing (DTP) is a process of printing ink with micronized dots using an inkjet printing machine to realize a designed pattern or image directly on a fabric. Digital textile printing has many advantages as follows. Firstly, it shortens the whole process time due to the elimination of screen plate manufacturing process. Secondly, it is an eco-friendly process that can reduce the environmental pollution such as waste-water. Finally, this printing method is suitable for small quantity batch production that can meet the needs of various consumers in a short time. Since DTP inks are printed with fine dots, a wider range of primary colors are required to widen the expression range of the printed pattern or image. Therefore, in this study we designed and synthesized new high-saturation deep blue color acid dyes to increase the expressive power of DTP ink. The synthesized dyes were based on modified triphenylmethine structure. In order to improve the low water solubility of this moiety, sulfonic acid groups were introduced. At the same time, the various dimeric structures were applied to improve the light resistance and optical properties of the dyes and they were compared with the commercial blue dyes. In addition, the ink formulation recipe was optimized using prepared dyes for high speed DTP.

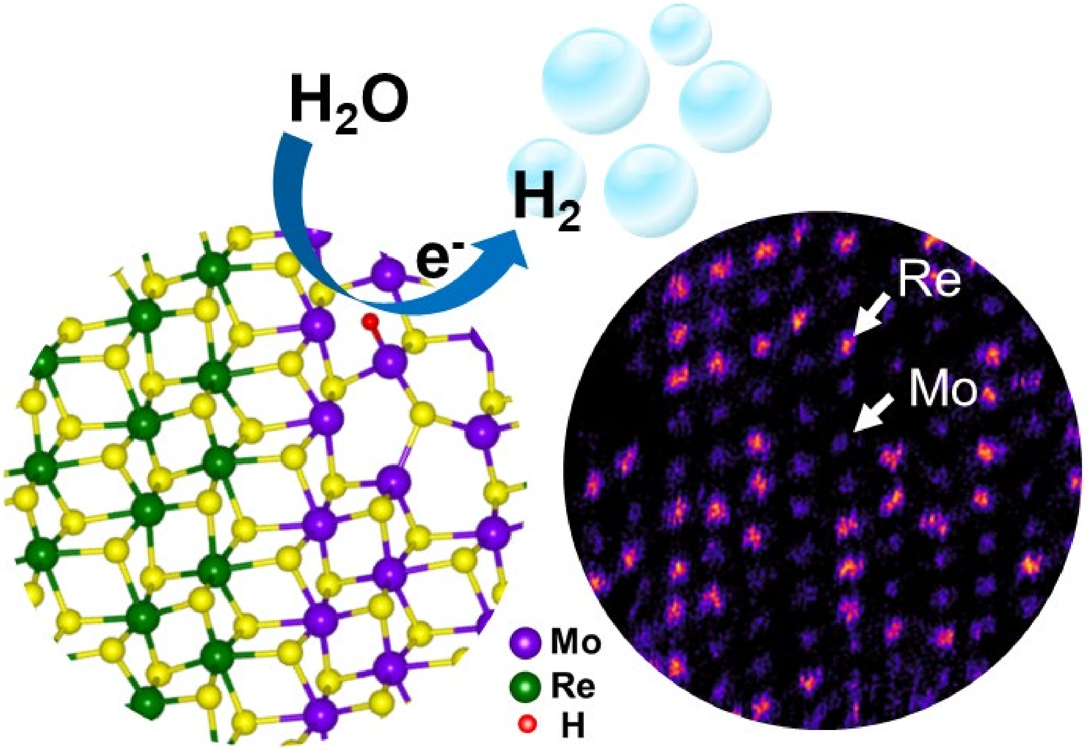
Poster Presentation : **MAT.P-463**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Anisotropic Alloying of Rhenium Molybdenum Sulfide Nanosheets for Electrochemical Hydrogen Evolution Reaction

In Hye Kwak, Ik Seon Kwon, Jeunghee Park*

Advanced Materials Chemistry, Korea University, Korea

Two-dimensional ReS_2 has recently attracted much attention as an excellent electrocatalyst for the hydrogen evolution reaction (HER). Herein, we synthesized $Re_{1-x}Mo_xS_2$ alloy nanosheets with the entire range of x using a hydrothermal reaction. High-resolution scanning transmission electron microscopy revealed anisotropic atomic distribution of the alloy phase, in which the Re and Mo atoms tend to segregate along a crystallographic axis. The transition from the triclinic phase (1T") ReS_2 to the monoclinic phase (1T') MoS_2 occurs at x = 50%, and hexagonal (2H) MoS_2 is produced as x increases further. $Re_{0.5}Mo_{0.5}S_2$ exhibited the best electrocatalytic performance toward HER in 0.5 M H_2SO_4, with a current of 10 mA cm^{-2} at an overpotential of 98 mV (vs. RHE) and a Tafel slope of 54 mV dec^{-1}. Extensive calculations using spin-polarized density function theory showed the 1T"→ 1T' phase transition of the bulk phase at x = 50%. At this composition, the most energetically stable configuration consists of separated MoS_2 and ReS_2 domains along the b axis, which agrees with the experimental results. The Gibbs free energy along the HER path indicates that the best performance at x = 50% is due to the formation of S-H or Mo-H (at S vacancies) on the MoS_2 domain.



$Re_{1-x}Mo_xS_2$ Nanosheets

Poster Presentation : **MAT.P-464**

Materials Chemistry

Zoom 8 WED 17:00~17:30

Adatom Doping of Transition Metals in $ReSe_2$ Nanosheets for Enhanced Electrocatalytic Hydrogen Evolution Reaction

Ik Seon Kwon, In Hye Kwak, Jeunghee Park*

Advanced Materials Chemistry, Korea University, Korea

Two-dimensional Re dichalcogenide nanostructures are promising electrocatalysts for the hydrogen evolution reaction (HER). Herein, we report the adatom doping of various transition metals (TM = Mn, Fe, Co, Ni, and Cu) in $ReSe_2$ nanosheets synthesized using a solvothermal reaction. As the atomic number of TM increases from Mn to Cu, the adatoms on Re sites become more favored over the substitution. In the case of Ni, the fraction of adatoms reaches 90%. Ni doping resulted in the most effective enhancement in the HER catalytic performance, which was characterized by overpotentials of 82 and 109 mV at 10 mA cm^{-2} in 0.5 M H_2SO_4 and 1 M KOH, respectively, and the Tafel slopes of 54 and 81 mV dec^{-1}. First-principles calculation predicted that the adatom doping structures (TMs on Re sites) have higher catalytic activity compared to the substitution ones. The adsorbed H atoms formed a midgap hybridized state via direct bonding with the orbitals of TM adatom. The present work provides a deeper understanding into how TM doping can provide the catalytically active sites in these $ReSe_2$ nanosheets.

Poster Presentation : **MAT.P-465**

Materials Chemistry

Zoom 8 WED 17:00~17:30

Improvement of Electrode Performance of MoS_2 Nanosheets upon Pillaring of Inorganic Nanocluster

Tae-Ha Gu, Seong-Ju Hwang[1,*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Department of Materials Science and Engineering, Yonsei University, Korea*

An effective way to improve the electrochemistry-related functionalities of MoS_2 material is developed by the intercalative hybridization with inorganic nanocluster. The pillaring with open tetrameric chromium hydroxide nanocluster leads to the remarkable improvement of the electrode performance of MoS_2, highlighting the usefulness of the present hybridization strategy in improving the electrode functionality of MoS_2 material. The enhanced electrode performance of the present nanohybrids can be ascribed to the formation of expanded interlayer structure, providing improved ion diffusion path, the stabilization of metallic 1T'-MoS_2 phase, the improvement of charge transfer kinetics, and the stabilization of open porous structure upon electrochemical cycling. Taking into account the universal applicability of the exfoliation—reassembling strategy for many kinds of transition metal dichalcogenide materials, the present study can provide an efficient way to improve diverse energy-related performances of these materials as electrodes, electrocatalysts, and photocatalysts.

Poster Presentation : **MAT.P-466**
Materials Chemistry
Zoom 8 WED 17:00~17:30

A Crucial Role of Interfacial Interaction in Improving Electro Catalyst Performance of Nanocomposites

Xiaoyan Jin, Seong-Ju Hwang[*]

Department of Materials Science and Engineering, Yonsei University, Korea

An efficient synthetic route to high-performance oxygen electrocatalysts is developed by employing conductive holey metal nitride nanotube (NT) with anion defects as a hybridization matrix for layered double hydroxide (LDH). The obtained holey metal nitride-LDH nanohybrid exhibits much higher electrocatalytic activity for oxygen evolution reaction (OER) than do the bulk metal nitride-LDH nanohybrid and the pristine LDH, underscoring the beneficial role of the holey NT morphology with significant crystal defects. The remarkable improvement of OER functionality upon the hybridization with holey metal nitride NT is attributable to the enhancement of interfacial electronic coupling, the increase of surface area and electrochemical active surface area, the improvement of OER kinetics, and the enhancement of charge transfer kinetics. The present study underscores that the defect control of conductive hybridization matrix can provide another effective way of optimizing the electrocatalyst functionality of hybrid materials via an enhanced interfacial electronic coupling.

Poster Presentation : **MAT.P-467**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Graphitic-Carbon Nitride Nanosheet as New Cationic Building Block for Bifunctional 2D Superlattice Nanohybrids

Nam hee Kwon, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

A pH-controlled g-C_3N_4 nanosheet (NS) is employed as an emerging cationic building block for MoS_2 NS to synthesize new class of superlattice nanohybrids of alternating graphitic-carbon nitride (g-C_3N_4)□transition metal dichalcogenide monolayers. The strong interfacial electronic coupling between interstratified g-C_3N_4 and MoS_2 NSs leads to the increase of structural stability and the formation of nitrogen defects. The intimate hybridization between electrocatalytically-active MoS_2 NSs and photocatalytically-active g-C_3N_4 NSs is quite effective in improving bifunctional catalyst performances for photocatalytic nitrogen fixation and electrocatalytic hydrogen evolution. Such a beneficial effect of hybridization is attributable to the promoted adsorption of protons, the provision of more active sites, the improvement of charge transfer kinetics, the increase of visible light absorptivity, and the enhancement of charge separation. The present study highlights that the application of g-C_3N_4 NS as a cationic building bock can provide an expanded library of multifunctional NS-based high-performance bifunctional catalysts.

Poster Presentation : **MAT.P-468**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Enhancement in Open-Circuit Voltages for Tin-based Perovskite Photovoltaics by Introducing a New Charge Transporting Layer

Myeongjeong Lee, Chung In*

School of Chemical & Biological Engineering, Seoul National University, Korea

Tin-based halide perovskite materials have been considered promising light absorbers for high-performance solar cells due to their absorption edges lying in the near-infrared region, low exciton binding energies, and high charge mobilities. However, solar cells based on these materials have shown poor open-circuit voltages (V_{OC}), mainly resulting from mismatched energy levels between a tin-based perovskite absorbing layer and charge transporting layers (CTLs). In this study, we show a reduced V_{OC} loss of tin-based perovskite solar cells by introducing a new fullerene-based CTL. We investigated the energy levels of a tin-based absorbing layer and various fullerene-based CTLs, and found our new CTL with the energy levels most suitable to a tin-based absorber. As a result, tin-based perovskite solar cells with a new CTL achieve a maximum power conversion efficiency of ~7% with the enhanced V_{OC} of ~0.65 V. This result highlights the importance of restructuring tin-based perovskite solar cells considering energy levels of device components.

126th General Meeting of the Korean Chemical Society
October 19(Mon)~21(Wed), 2020, Online Meeting

Poster Presentation : **MAT.P-469**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Fabrication of Molecular Tunnel Junction Arrays via Direct Printing of Liquid-Metal Microelectrode

Seo Eun Byeon, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

The printability remarkably expands the application range of electronics, particularly for large-area electronic displays, sensors, solar cells, antennas, and transistors. Printed electronics allows cost-effective and high-throughput fabrication of standardized devices with various shapes and patterns. Direct printing of conductive material on self-assembled monolayers can potentially offer a route to unprecedented merging of molecular electronics with printed electronics. Given that monolayers are extremely sensitive to structural changes at the atomic level and easily damaged by external stimuli, it is a significant technological challenge to make conformal and uniform top-contacts at the delicate hydrophobic surface of organic monolayers via direct printing while maintaining reproducibility and reliability of tunneling performance and high yields of working devices. This presentation shows an approach to fabricate arrays of molecular tunnel junctions via automated direct printing of liquid-metal microelectrode comprising eutectic gallium-indium onto self-assembled monolayers (SAMs) of n-alkanethiolates. Our printing system enables formation of 350 tunneling junctions on 2 cm × 2 cm template-stripped chip (2,800 junctions per batch). Under an optimized condition, liquid metal (eutectic Ga-In) microelectrodes were evenly printed, which led to uniform geometrical contact area of ~4.7×10^3 μm^2 in individual junctions. The resulting junctions exhibited high yields of working junctions (> 80%) and narrow single log-normal distributions ($\sigma_{\log|J|} = 0.2 – 0.5$) of tunneling current density (J, A/cm^2). There were no noticeable variations in tunneling decay coefficient ($\beta = 0.95 \times 0.02$ nC^{-1}) and charge injection current density ($J_0 = 10^{3.2\pm0.2}$ A/cm^2) between electrodes and batches.

Poster Presentation : **MAT.P-470**
Materials Chemistry
Zoom 8 WED 17:00~17:30

The Synthesis and Characterization of Perovskite Nano Crystals for Inkjet-printed Color Conversion Layer of High Color Purity

Sang Yoon Lee, Lee Geonho[1], Seong Hyun Jang[2], Jun Choi[3,*]

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[2]*Human Institute of Industrial Technology Convergen, Korea Institute of Industrial Technology, Korea*
[3]*Korea Institute of Industrial Technology, Korea*

Recently, all-inorganic halide perovskites have attracted great attention as optoelectronic devices such as solar cell, LED, Photo detector, and laser. But the massive defects reduce their optical properties and consequently limit the device performance. Thus, we synthesized all inorganic perovskite nanocrystals by hot injection method with SCN passivation for the wide-color gamut low-cost displays. The SCN^- ion from NH_4SCN passivated the perovskite nanocrystals to reduce the surface defect density and increase the air stability. The prepared perovskite nanocrystal solutions were formulated into the ink-jet printable homogeneous inks and uniformly coated as the color conversion layers for the perovskite nanocrystal/blue-OLED hybrid display. The inkjet printing exhibits a simple process, low cost, high degree of automation, and selective patterning without using a mask. Some large-area display manufacturers are already today employing inkjet printing to fabricate future high-resolution organic LEDs. However, there are not many cases reported on perovskite LEDs yet. Through these processes, we confirmed the excellent photophysical properties of the fabricated perovskite nanoparticle inks and the color conversion layers for the perovskite nanocrystal/blue-OLED hybrid display.

Poster Presentation : **MAT.P-471**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Critical evaluation of a model-based estimation of monolayer coverage in porous materials: a case study of solid-like H_2 adsorption

SungHyun Yun, **Yongchul Chung***

Chemical & Biomolecular Engineering, Pusan National University, Korea

Recently, solid-like adsorption of hydrogen on nanoporous carbon material at 77 K has been experimentally observed, but the origin of high-density hydrogen adsorption remains to be elusive to date. In this work, GCMC simulations were carried out on different metal-organic frameworks (MOFs) and graphite-sheet pore models to elucidate the critically evalute the model-based approach to estimate the monolayer coverage in porous materials. The adsorbed hydrogen densities obtained from the simulation were compared with densities obtained by fitting a model equation to simulated excess isotherm. We find that the model-based estimation of the density of adsorbed hydrogen overestimates the true density of adsorbed hydrogen obtained from the simulation by more than 50%. We discuss the origin of the discrepancies between the model-based approach and molecular simulation.

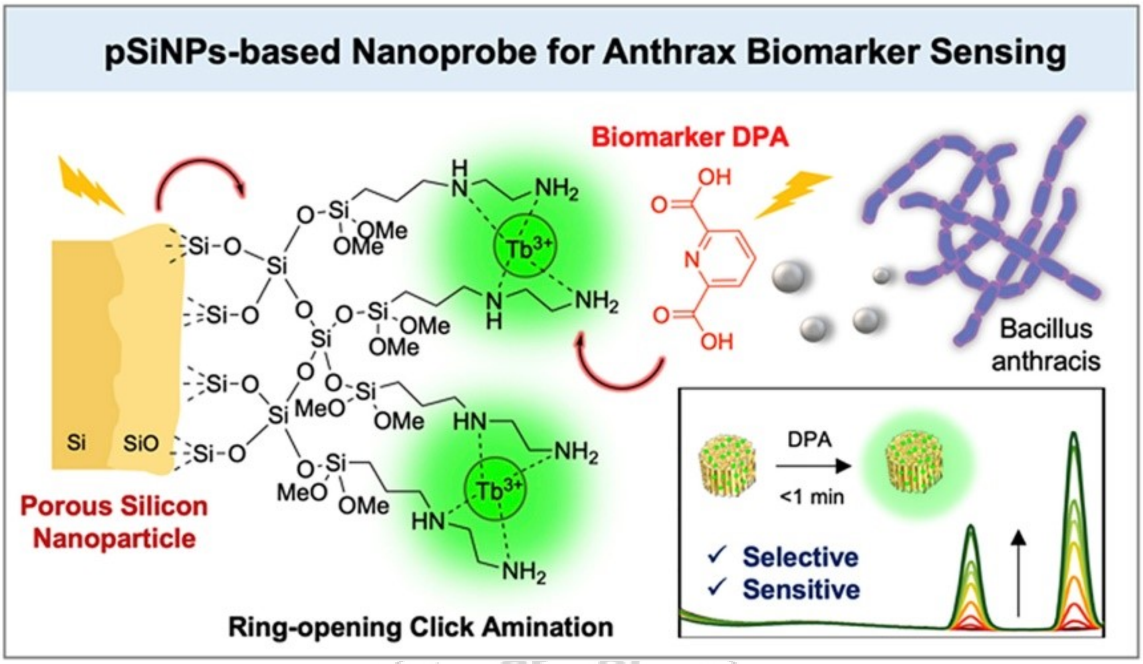
Poster Presentation : **MAT.P-472**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Porous silicon nanoprobe for the detection of anthrax biomarker and its practical applications

Yuna Jung, Dokyoung Kim[1,*]

Department of Biomedical science, Kyung Hee University, Korea
[1]College of Medicine, Kyung Hee University, Korea

Anthrax is a severe contagious disease caused by Bacillus anthracis (B. anthracis) that has long been threatened in human life as a biological weapon. Polymerase chain reaction (PCR) or Gram-staining is generally used to detect these bacteria, but it is difficult to sense biomarkers in situ and in real-time. In order to overcome those limitations, we introduced porous silicon (pSi) nanoprobe (named; pSiNPs-Tb) for detecting dipicolinic acid (DPA), which is a representative biomarker of anthrax spores, and demonstrated its availability. Due to the unique properties of pSi, such as large surface area and internal pores, the pSi has been adopted for developing optical devices and drug delivery systems (DDS). In this study, we developed a pSi-based nanoprobe that capable of real-time detection of biomarkers of anthrax by modifying the surface of pSi nanoparticles through a ring-opening click amination and terbium ion (Tb3+) grafting. The nanoprobe exhibited selective fluorescence turn-on response toward DPA, and manifested high sensitivity and fast response time. A dual antenna effect from DPA/pSiNPs to terbium ions amplified its sensing capacity toward DPA and its sensing property was compared with non-porous silica nanoparticles. In the practical application based on a paper-strip, the excellent real-time on-site detection capability was demonstrated. On the basis of our study results, we believe that the nanoprobe could be applied to diverse spore-derived disease as a diagnostic tool.


pSiNPs-based Nanoprobe for Anthrax Biomarker Sensing
Biomarker DPA
OH
O
N
O
OH
Bacillus anthracis
Si
SiO
Porous Silicon Nanoparticle
Si-O
O-Si
OMe
Tb3+
NH2
H
N
MeO
HN
Ring-opening Click Amination
DPA
<1 min
✓ Selective
✓ Sensitive

Poster Presentation : **MAT.P-473**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Enhanced Thermoelectric Performance in eco-friendly Coated Grain boundary system

Minju Lee

Chemistry & Nanoscience , Ewha Womans University, Korea

Recently, composites comprising grain boundaries with excellent thermoelectric performance due to a short mean free path and energy filtering effect of phonons have attracted much attention. In this study, we developed a strategy for grain boundary containing new nanocomposite using surface coated nanoparticles prepared by a cation exchange method. Cu was used as an eco-friendly coating element instead of Cd in our previous CdTe grain boundary contained SnTe composite to overcome toxicity problem of Cd. Cu was chosen as a coating metal by considering following two factors: First, solubility product Ksp was considered as a driving force of the cation exchange process on surface of SnTe particles. It was expected that metals in chalcogenide with a Ksp lower than Sn in SnTe would spontaneously undergo a cation exchange process to form a surface coating layer of Cu2Te on SnTe. Second, Pearson's hard/soft-acids/bases (HSAB) theory was used as a tool to predict the interaction among solvents, ligands, and ions. If host SnTe particles are surrounded by ligands and can form a more stable acid–base pair with the solvent and ligand, the host cations can be removed and replaced at the surface. Therefore, it is important to understand the interaction between the ligand and surface ions. Using these two thermodynamic concepts, Cu and Ag were selected as promising coating metal candidates. Consequently, the thermoelectric figure of merit of the SnTe composite with Cu2Te coated grain boundaries was improved by about 80% compared to SnTe. In this eco-friendly material, the thermal conductivity is reduced and the power factor is enhanced resulting in a high zT value of 1.4 at 850 K.

Poster Presentation : **MAT.P-474**
Materials Chemistry
Zoom 8 WED 17:00~17:30

2D Organic-Inorganic Hybrid Tin (II) Iodide Perovskites

So-Hyeon Yang, Youngmee Kim, Sung-Jin Kim*

Department of Chemistry and NanoScience, Ewha Womans University, Korea

As interest in 3D perovskites AMX3 with high power conversion efficiency over than 20%, there are many researchers studying on organic-inorganic lead halide perovskites. However, there are two major problems: lead toxicity and moisture stability. One of the many ways to overcome this stability problem is to lower the dimensionality of the crystal structure to 2D and 1D. To solve the lead toxocity, replace lead (II) ion with tin (II) ion. In this study, we synthesized two-dimensional organic-inorganic tin (II) iodide perovskite hybrids to reduce lead toxicity and increase moisture stability. We succeeded in discovering new compounds by studying how to adjust the dimensionality of the crystal structure. They have capability of tuning structures and optical properties. Our new 2D materials are formulated as (4AMP)SnI4, (4AMP)Sn3I8, and (MA)2Sn3I8. (4AMP)SnI4 is consisted of single layers containing corner-sharing SnI6 octahedra and each single layer is separated by (4AMP)2+ organic cations. (4AMP)Sn3I8 and (MA)Sn3I8 are three-layer-thick perovskites divided by (4AMP)2+ cations and filled with 2(MA)+ cations, respectively. Crystal structures and optoelectronic properties of these 2D organic-inorganic hybrid tin(II) iodide perovskites will be discussed.

Poster Presentation : **MAT.P-475**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Anisotropic Two-Dimensional SiAs for High-Performance UV-Visible Photodetectors

Doyeon Kim, Jaemin Seo[1], In Hye Kwak[2], Ik Seon Kwon, Kidong Park[3], Jeunghee Park[1,*]

Advanced Materials Chemistry, Korea University, Korea
[1]*Department of Materials Chemistry, Korea University, Korea*
[2]*Micro Device Engineering / Microdevices, Korea University, Korea*
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Binary IV-V group (IV = Si, Ge and V = P, As) compounds have attracted much attention as new class of anisotropic 2D materials due to their monoclinic or orthorhombic unit cells. Herein, we synthesized 2D SiAs bulk crystal using a solid-state reaction, and a few layered nanosheets via a mechanical exfoliation of bulk crystal. The strong in-plane anisotropy of phonon vibration has been investigated using angle-resolved polarized Raman spectroscopy. The anisotropic electrical properties of SiAs nanosheets were examined by fabricating a top-gate field effect transistor on the SiO2/Si substrate. Furthermore, SiAs nanosheet exhibit a high photosensitivity (on/off ratio = 10^2) with a strong anisotropic ratio in UV-visible range; anisotropic factors of 5.8 at 514 nm and 2 at 325 nm. This work lays the foundation and ignites future research interests in anisotropic group IV–V materials.

Poster Presentation : **MAT.P-476**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Chalcogen-Vacancy Group VI Transition Metal Dichalcogenide Nanosheets for Solar-Driven Photoelectrochemical Hydrogen Evolution

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Solar-driven photoelectrochemical water splitting has been considered as the most promising technology for generating hydrogen energy. Transition metal dichalcogenide (TMD) compounds have currently attracted tremendous attention due to their outstanding ability towards the catalytic water-splitting hydrogen evolution reaction (HER). Herein, we report the facile synthesis of chalcogen-vacant transition metal dichalcogenide (TMD, i.e., MoS2, MoSe2, WS2, and WSe2) nanosheets directly on the pre-grown Si nanowire (NW) arrays. The TMDs exhibited excellent electrocatalytic HER activity in in 0.5 M H2SO4, with a current of 10 mA cm-2 at an overpotential of 100 mV (vs. RHE) and a Tafel slope of 50 mV dec-1. Photocathodes consisted of Si-TMD NW arrays exhibit excellent PEC performance; the photocurrent reaches to 30 mA cm-2 (at 0 V vs. RHE) and the onset potential is 0.2 V under AM1.5 condition. The stability is 90% for 12h with high quantum efficiency of hydrogen generation (avg. 90%). Detailed structure analysis shows the chalcogen vacancies play a major role in enhancing the PEC performance. The efficient catalytic activity toward HER protect the self-oxidation of Si NW and cause this enhanced PEC performance, promising efficient water-splitting Si-based PEC cells.

Poster Presentation : **MAT.P-477**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Phase Controlled Growth of Cd_3As_2 Nanowires

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The bottom-up synthesis process often allows the growth of metastable phase nanowires instead of the thermodynamically stable phase in the bulk counterpart. Herein, we synthesized single-crystalline Cd_3As_2 nanowires with a controlled three-dimensional Dirac semimetal phase using a chemical vapor transport method. Cd_3As_2 nanowires were selectively grown with three different phases such as the stable body centered tetragonal (bct) phase and two metastable primitive tetragonal (pt) phases. The conversion between three phases was controlled by the growth temperature (320–450 °C). The growth direction of Cd_3As_2 nanowires depends on the phase; [1-10] for bct phase, while [1-10] or [100] for pt phases. We fabricated field effect transistors and photodetector devices, showing the nearly same electrical and photoelectrical properties for three phases. Differential conductance measurement showed that the n-type Cd_3As_2 nanowires had an electron mobility of 2×10^4 cm^2/V s at 10 K. Negative photoconductance was first observed, and the photoresponsivity reached 3×10^4 A/W. The negative photoconductance is ascribed to the surface defects acting as trap sites for the photogenerated electrons.

Poster Presentation : **MAT.P-478**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Simple and Rapid Synthesis of Highly Efficient Cesium Lead Halide Perovskite Nanocrystals by Ultrasonication Method

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Perovskite has high potential as a next-generation display light emitting material with bright, low-cost, tunable emission wavelength, high photoluminescence quantum yield, and narrow full width at half maximum. However, there are the following problems for perovskite to be commercialized. First, the stability of oxygen and moisture in the air is poor. Second, massive surface ionic defects reduce their optical properties. Finally, conventional methods such as hot injection method and ligand-assisted re-precipitation technology (LARP) are difficult to manufacture on a large scale due to complex conditions and long synthesis time. In this study, we introduce an ultrasonication method (USM) that improves the stability of $CsPbX_3$ perovskite nanocrystals and is optimized for rapid and mass-producible synthesis. The USM was quick and simple to synthesize in minutes by putting all the precursors in one-pot. Here, SCN^- passivated defects with the introduction of ammonium thiocyanate. As a result, stability was improved and photoluminescence quantum yield was greatly enhanced.

Poster Presentation : **MAT.P-479**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Enhancing n-type thermoelectric performance of polycrystalline SnSe by PbSe alloying and Halogen doping

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Thermoelectric (TE) materials enable direct and reversible transition between heat and electricity, thereby a promising means of renewable energy technology. Single crystal SnSe is a representative thermoelectric material with high performance over temperature range of 773-923 K. The high TE performance of SnSe is originated from its anisotropic crystal structure and multiple electronic band structure. Despite its high TE performance, practical TE applications of single crystal SnSe are limited because synthesizing sizable, high quality single crystal SnSe is expansive and labor-intensive process. However, n-type polycrystalline SnSe exhibits inferior performance to its single crystalline counterpart yet, because it is hard to stabilize n-type carrier in the polycrystalline n-type SnSe. Here we report our synthesis of n-type polycrystalline SnSe system by PbSe alloying and chlorine doping, namely, $Pb_xSn_{1-x}Se_{0.98}Cl_{0.02}$ ($0 \leq x \leq 0.2$). By optimizing PbSe alloying fraction, electrical conductivity of PbSe alloying and chorine doped SnSe were significantly enhanced, resultantly improving power factor. It also reduces thermal conductivities due to point defect scattering of heat-carrying phonon, leading to thermoelectric figure of merit (ZT) of ~1.4 at 823K for optimized sample.

Poster Presentation : **MAT.P-480**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Investigation of the structural and optoelectronic properties of Ga_2S_3 Nanowires.

<u>Jaemin Seo</u>, Kidong Park[1], Doyeon Kim[2], In Hye Kwak[3], Ik Seon Kwon[2], Jong Hyun Lee[2], Jeunghee Park[*]

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Gallium sesquisulfide (Ga_2S_3) is unexplored wide band gap semiconductor materials, having a defective zinc blende-like structure in which one third of the cationic sites are vacant. There are several polymorphs that differ in the arrangement of the atoms and vacancies, which make difficult to synthesize pure phase. In the present work, we synthesized the Ga_2S_3 nanowires (NWs) using a catalyst-assisted chemical vapor transport method. To our best knowledge, it is the first report of achieving completely pure monoclinic and the coexisting monoclinic-hexagonal phase in Ga_2S_3 NWs. Utilizing a temperature-dependent synthetic approach, Ga_2S_3 NWs were selectively grown. The growth direction of Ga_2S_3 NWs was changed $[001]_M//[000\text{-}1]_H \rightarrow [010]_M//[\text{-}2110]_H \rightarrow [\text{-}3\text{-}31]_M//[0\text{-}110]_H$ with decreasing growth temperature in the range of 900K<T

Poster Presentation : **MAT.P-481**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Multiscale computational investigation of all-silica zeolites for simultaneous removal of H_2S and CO_2 for natural gas upgrading

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Despite the recent surge in the production of natural gas in the North American and the World Wide, a significant portion of the global gas reserves continues to remain untapped due to the sour nature of these reserves due to the high concentration of H_2S and CO_2 in the produce natural gas. Removal of H_2S and CO_2 is typically carried out based on the amine-based absorptive separation, followed by a Claus process. Still, the high concentration of H_2S makes the separation uneconomical, which calls for the development of new and innovative approaches to separate the high concentration of H_2S and CO_2 from the natural gas. Toward this end, adsorptive separation based on zeolites has been proposed in the literature to achieve separation of H_2S or CO_2 from natural gas. Several computational screening studies on the experimentally realized zeolite structures have discovered some zeolite materials for the adsorptive H_2S removal under humid conditions. Still, these materials typically exhibit low CO_2 uptake due to the competitive adsorption of water over CO_2 in these materials. In this work, we explore the idea of layering the adsorber with different zeolites to achieve the simultaneous removal of H_2S and CO_2 under both humid and dilute conditions. For this purpose, we combined process-level modeling with the high-throughput grand canonical Monte Carlo (GCMC) computational screening on experimentally reported all-silica zeolite database.

Poster Presentation : **MAT.P-482**

Materials Chemistry

Zoom 8 WED 17:00~17:30

Observing extending PL lifetime by raising temperature of organic–inorganic hybrid perovskite materials via TCSPC lifetime measurement

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Light emitting materials which emits long lived photoluminescence can be applied to bio imaging agent, light-emitting chemical sensor and light-emitting device and photovoltaics. Among these materials, metal halide organic-inorganic hybrid perovskite materials have got attention due to triplet exciton that involves photophysical process. To investigate long lived exciton of hybrid materials, we introduce 1,8-naphthalimide based aromatic ammonium cations to Ruddlesden-Popper type lead halide perovskite lattices. In their film samples, we observed photoluminescence spectra that has large Stokes-shift and specific vibrational state. The emission result from phosphorescence of the aromatic organic cation although only organic cation thin film emitted small Stokes shift and non-specific vibrational spectra compared to perovskite film. By measuring photoluminescence lifetime measurement, PL decay of low energy was extended to millisecond range. In addition, unlike other phosphorescence light emitting materials, PL lifetime of the film increased as raising the temperature of the film because the energy gap of organic cation between room temperature and low temperature was too small to up-convert lower energy to higher energy by thermal energy. This phenomenon gives us an example for interaction metal halide materials and up-conversing organic chromophore.

Poster Presentation : **MAT.P-483**
Materials Chemistry
Zoom 8 WED 17:00~17:30

Thermoelectric Properties of Chromium-doped Cu-Sn-S Compound

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The thermoelectric materials have attracted attraction due to needs for potential renewable energy source. The efficient of thermoelectric generator can be evaluated by the figure of merit , $ZT=S^2\sigma T/\kappa$, where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature and κ is the thermal conductivity.Among the various kinds of thermoelectric materials, sulfide materials are regarded as a promising eco-friendly TE material due to their earth abundant, low-cost and non toxic elements. The Cu_2SnS_3 material selected because there is a 3-dimmensional conductive network between Cu 3d orbitals and S 3p orbitals. In the band structure of Cu_2SnS_3, the upper valence bands composed of hybrid Cu 3d orbitals and S 3p orbitals while containing no evident contribution from Sn atoms. We pelletized chromium-doped Cu_2SnS_3 with hot pressing. The crystal structure investigated monoclinic phase by X-ray diffraction. In the monoclinic structure of Cu_2SnS_3, there is a 3-dimensional conductive lattice network with ordered atom arrangement.We will measure the thermoelectric properties of the chromium-doped Cu_2SnS_3 by ZEM-3 equipment (Ulvac-Riko) and NETZSCH LFA 457 MicroFlash^{TM}.

Poster Presentation : **MAT.P-484**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Plasmon-Induced polymerization of Poly(Acrylic acid) on Gold Nanoparticles

Jeonghyeon Lee, Youngsoo Kim*, Hyeonji Kim

Department of Chemistry, Yeungnam University, Korea

Polymeric/gold nanocomposites are receiving great interest in chemistry, biochemistry, and material science because it can be applicable to many academic and industrial fields like liquid crystal, polarized film, catalysts, and drug-delivery, and so on. Especially, gold nanoparticles have been highlighted in the field of catalysis and drug-delivery due to the catalytic ability in the nanoscale regime, and biocompatibility. Also, gold nanoparticles have a signature to generate thermal energy in the vicinity of nanoparticles through phonon-phonon scattering, resulting from light-to-matter interactions. Such photothermal property of gold nanoparticles can be a beneficial strategy for synthesizing polymeric materials onto the gold nanoparticles. Here, we directly synthesized Poly(Acrylic acid)@gold nanocomposite through photothermal effect of gold nanoparticles under visible light. The optical property of products was identified with a UV-Vis spectrophotometer and the morphology and the chemical information of the products were characterized by TEM, NMR, TGA, and FT-IR.

Poster Presentation : **MAT.P-485**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Particle Size-Dependent Electron Transfer Kinetics on Plasmonic Au Photocatalyst

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Plasmonic gold nanoparticles are drawing attention as a promising material for visible-light-driven photocatalysts due to their strong light absorption in the visible light region. Recently, much researches for the plasmonic photocatalysts has been reported that is for electron transfer kinetics and to drive important chemical reactions such as CO_2 reduction and N_2 fixation. Such researches, the size of the gold nanoparticles used were fixed around 13 nm in diameter, which is synthesized by the Turkevich method. The electron transfer kinetics can be tuned by the ability of light absorption. As the size of plasmonic gold nanoparticles grows, the absorption cross-section could be reduced because of the contribution of the scattering effect. Therefore, we focused on the change in electron transfer rate with varying the size of gold nanoparticles (~13 nm, ~20 nm, ~25 nm, ~35 nm). To investigate the photocatalytic activities on different sizes of gold nanoparticles, we employed Ferricyanide(Fe^{3+})/Ferrocyanide(Fe^{2+}) redox couple as a colorimetric indicator. To find reaction kinetics by different sizes of gold nanoparticles, we conducted power-dependent and wavelength-dependent experiments and monitored the reaction conversion as a function of irradiation time.

Poster Presentation : **MAT.P-486**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Plasmon-Induced Intramolecular Carbon-Carbon Bond Formation with Au Nanoparticles

Juhee Ha, Youngsoo Kim*

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The homo- and the hetero-coupling reaction is one of the crucial and important synthetic strategies to construct a new carbon-carbon bond in the final organic product. Especially, these types of coupling reactions have been routinely employed in the preparation of pharmaceuticals and conjugated polymer synthesis. So far, many notable coupling reactions required transition metal catalysts like Pd, Ni, and Cu as a catalyst, and high reaction temperatures and toxic chemicals employed to achieve the new product. To overcome harsh reaction conditions and environmental issues in conventional synthetic methods, alternative synthetic strategies to form a carbon-carbon bond have been diversely proposed. Among those new ways proposed, the photocatalysis technique which uses only catalysts and light can be a reasonably unique approach because it requires mild reaction conditions (temperature and time) and less toxic chemicals. For the past decades, gold nanoparticles have been receiving great attention as photocatalyst because of unique optical property and catalytic activity at the nanoscale. Thus, we employed gold nanoparticles and visible light for the reaction of C-C coupling. In this study, we conducted a carbon-carbon single bond formation under the condition of room temperature and non-toxic chemicals with aryl halide, organoboron species, and base. Gold nanoparticles were characterized by TEM and UV-Vis spectrophotometer, and the final products were characterized by NMR and GC and GC-MS. On the basis of the fact, we confirmed that the biphenyl was synthesized by plasmonic gold catalysts, and the phenol and benzene were produced as a by-product.

Poster Presentation : **MAT.P-487**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Hot Electron Transfer Kinetics in Aggregation-Induced Space of Gold Nanoparticles

Jueun Bae, Youngsoo Kim[*]

Department of Chemistry, Yeungnam University, Korea

Noble metal nanoparticles, i.e., Au, Ag, and Cu, have been received increasing attention as a visible light-driven photocatalysts due to their unique optical property arising from localized surface plasmon resonance (LSPR). However, these types of photocatalysts have inherent limitations that the rate of recombination of excited electrons and holes is too fast so that these charge carriers cannot easily participate in chemical reactions. As a consequence, the reaction rate in plasmonic photocatalyst is limited by the diffusion rate of chemical species to the photocatalysts, resulting in showing a slower reaction rate. To enhance the rate of reaction in plasmonic photocatalysts, it can be one of the key ideas that either the migration length of excited electrons or diffusion length of reaction species needs to be shortened. In this study, we made a confided space that can aid to reduce the distance between photocatalysts and the reaction species through surface engineering on nanoparticles. We will compare the reaction kinetics in plasmonic photocatalysis between the colloidal nanoparticle system and the nanoreactor system and will endeavor to find mechanistic insight in photochemical electron transfer in a nanoscale reactor.

Poster Presentation : **MAT.P-488**
Materials Chemistry
Zoom 8 WED 17:30~18:00

High stability Li-halide based Li_3MCl_6 electrolyte with high ionic conductivity for all-solid-state batteries

<u>Sunggeun Lee</u>, Myoungho Pyo[1,*]

Department of Printed Electronics Engineering, Sunchon National University, Korea
[1]*Department of Printed Electronics Engineering, Suncheon National University, Korea*

To solve the recently emerged battery safety issues, all-solid batteries are the best alternative. Many solid electrolytes have been studied for all-solid-state batteries, and among them, sulfur-based electrolytes have excellent ionic conductivity. However, most of the sulfur-based electrolytes show extreme sensitivity to air and moisture, and cannot satisfy both characteristics of high ionic conductivity and high stability required for commercialization of all-solid batteries. To solve this, a Li-halide-based electrolyte has been proposed. Li-halide electrolyte, Li_3InCl_6 shows high stability in dry air and even when it exposed to moisture, it can recover the electrochemical properties by heating. For checking the multivalent materials substitution effect, Pb, Zr and Nb are doping on the Li_3InCl_6 with two different synthesis method. The crystal structure of the synthesized materials was characterized by XRD. And electrochemical properties was characterized by cold pressed pellet zig-cell.

Poster Presentation : **MAT.P-489**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Visible-Light-Promoted Intramolecular C-N Bond Formation Using Plasmonic Au and Au@Pd Core-Shell Nanoparticles

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Nitrogen-containing organic compounds are extensively found in bioactive natural products and pharmaceutical materials, and those materials have been highlighted the importance in the pharmaceutical market and electronics industry. Especially, Carbazole and its derivatives, which is one of the great examples of aromatic heterocyclic compounds, are also receiving importance due to their versatile medicinal uses and optoelectronic abilities. Among diverse synthetic strategies for Carbazole synthesis, one possible way is the C-N bond formation in a molecule. While much effort to construct the intramolecular C-N bond formation has been continued, C-N bond formation under mild condition is still a challenging task for organic synthetic chemists. In the past decades, various groups conducted amination reactions under mild and convenient conditions using transition metal-catalysis like Pd, Cu, and Ru. However, those protocols still have inevitable problems that use high temperatures, toxic solvent, and long reaction time, and so on. Herein, we conducted the intramolecular C-H bond amination of N-benzenesulfonyl amidobiphenyl, using only light and plasmonic Au and Au@Pd core-shell nanoparticles as photocatalysts in the absence of hazardous solvent. Based on the NMR and GC-MS results, we found that the cleavage of N-S bond of N-benzenesulfonyl amidobiphenyl and the formation of C-N bond has occurred simultaneously. Consequently, we realized that the 9H-Carbazole was synthesized in the presence of plasmonic Au nanoparticles and visible light. We expect that our results will be a promising approach to drive amination in terms of green chemistry.

Poster Presentation : **MAT.P-490**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Realizing Exceptionally High Average Power Factor and Thermoelectric Figure of Merit in n-type PbSe by Dual Incorporation of Cu and Te

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Simultaneously improving power factor and ZT values has been one of the hardest challenges in thermoelectrics regardless of systems of interest. Here we report that new n-type thermoelectric system CuxPbSe0.99Te0.01 (x = 0.0025, 0.004, and 0.005) exhibiting record-high average ZT of ~1.3 from 400 to 773 K ever reported for any n-type polycrystalline materials including the state-of-the-art PbTe. We concurrently alloy Te to the PbSe lattice and introduce excess Cu to its interstitial voids. Atom probe tomography analysis confirmed a strong attraction between interstitial Cu and Te atoms in the lattice. It increased carrier concentration without damaging its mobility and the consequently improved electrical conductivity. This interaction also increases effective mass of electron in the conduction band according to the first principle calculation, raising the magnitude of Seebeck coefficient without diminishing electrical conductivity. Resultantly, Cu0.005PbSe0.99Te0.01 attains exceptionally high average power factor of ~27 μW cm−1 K−2 from 400 to 773 K with a maximum of ~30 μW cm−1 K−2 at 300 K, which is the highest among all PbSe-based materials. Its ~23 μW cm−1 K−2 at 773 K is even higher than ~21 μW cm−1 K−2 of the state-of-the-art n-type PbTe. Interstitial Cu atoms induce the formation of coherent nanostructures. They are highly mobile under electron beam irradiation accompanied by local heating, consequently displacing Pb atoms from the ideal octahedral center and severely distorting the local microstructure. This significantly depresses lattice thermal conductivity to ~0.2 Wm−1 K−1 at 773 K below the theoretical lower bound. The multiple effects of the dual incorporation of Cu and Te synergistically boosts a ZT of Cu0.005PbSe0.99Te0.01 to ~1.7 at 773 K.

Poster Presentation : **MAT.P-491**
Materials Chemistry
Zoom 8 WED 17:30~18:00

New 2D Metallic ZnSb with High Carrier Mobility from 3D Semiconducting ZnSb

Weiqun Lu, Chung In[1,*]

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[1]*School of Chemical & Biological Engineering, Seoul National University, Korea*

Since the pioneering work in 2004, graphene, consisting of atomically thin layers of sp2-hybridized carbon atoms, offers a fascinating platform to study the structure–property relationships. Motivated by the success of graphene, alternative emerging members are constantly being explored for many promising applications. Herein, we have meticulously explored the phase evolution of three Zintl zinc antimonides. Particularly, 2D ZnSb with the sp2 hybridization features weak van der Waals forces in the interlayer interactions, endowed with exfoliation availability. The stacking configuration of constituent atoms captured by the aberration-corrected STEM study also implies its exfoliatable behavior. Meanwhile, 2D ZnSb achieves high carrier mobility up to ~468 cm2 V−1 s−1 at room temperature, exceeding 5 times that of 3D ZnSb, comparable to or even superior to those of the other representative 2D materials. Electronic band structures directly visualized by ARPES measurements identify its metallic nature. The work presented here sheds light on developing new unpredictable 2D phases via stepwise topotactic pathways with extraordinary physical properties.

Poster Presentation : **MAT.P-492**
Materials Chemistry
Zoom 8 WED 17:30~18:00

High Voltage Dentrite-free Lithium Metal Battery Electrolyte Utilizing Adiponitrile Single Solvent and NO2BF4 as Electrolyte Additive

Manasi Mwemezi

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Abstract Adiponitrile (ADN), which generally exhibits high anodic stability, is a troublesome solvent in a lithium electrolyte due to an inability to form a robust and stable solid electrolyte interface (SEI) on an anode, which hinders its application as single solvent in lithium ion batteries (LIBs). In this work, we describe addition of small quantities of nitronium tetrafluoroborate (NO2BF4) to an ADN based Li electrolyte that resulted in three major benefits. Firstly, NO2BF4 distinctively modified the otherwise unstable SEI, by forming a robust thin Li2O/LiF laden SEI capable of mitigating relevant detrimental surface side reactions at the electrode, therefore enabling remarkably stable and reversible electrochemical plating/stripping of Li on metallic substrates and/or Li, without the need for a co-solvent. Secondly, in contrast to typical indications of dendritic nucleation in carbonate electrolytes, effective suppression of dendritic growth and stable cycling was evidenced in an no2bf4 containing ADN electrolyte. Thirdly, the above achievements were realized with no negative effect of the additive on the anodic stability of the electrolyte, which provided impetus to test high voltage operation at 20 □C. Lithium battery incorporating Li anode/LiMn2O4 assembled using the additive containing electrolyte displayed good reversible capacity and cyclic retention (100 mAhg-1 at 1C for 200 cycles) and when tested at potentials >5.6 V at high C rates (12C), showed stable capacity (90.7 mAhg-1), and remarkable cooperation of Li anode and anodic suppression in anodic electrolyte decomposition.

High Voltage Dentrite-free Lithium Metal Battery Electrolyte Utilizing Adiponitrile Single Solvent and NO_2BF_4 as Electrolyte Additive

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Abstract

Adiponitrile (ADN), which generally exhibits high anodic stability, is a troublesome solvent in a lithium electrolyte due to an inability to form a robust and stable solid electrolyte interface (SEI) on an anode, which hinders its application as single solvent in lithium ion batteries (LIBs). In this work, we describe addition of small quantities of nitronium tetrafluoroborate (NO_2BF_4) to an ADN based Li electrolyte that resulted in three major benefits. Firstly, NO_2BF_4 distinctively modified the otherwise unstable SEI, by forming a robust thin Li_2O/LiF laden SEI capable of mitigating relevant detrimental surface side reactions at the electrode, therefore enabling remarkably stable and reversible electrochemical plating/stripping of Li on metallic substrates and/or Li, without the need for a co-solvent. Secondly, in contrast to typical indications of dendritic nucleation in carbonate electrolytes, effective suppression of dendritic growth and stable cycling was evidenced in an no2bf4 containing ADN electrolyte. Thirdly, the above achievements were realized with no negative effect of the additive on the anodic stability of the electrolyte, which provided impetus to test high voltage operation at 20 °C. Lithium battery incorporating Li anode/$LiMn_2O_4$ assembled using the additive containing electrolyte displayed good reversible capacity and cyclic retention (100 $mAhg^{-1}$ at 1C for 200 cycles) and when tested at potentials >5.6 V at high C rates (12C), showed stable capacity (90.7 $mAhg^{-1}$), and remarkable cooperation of Li anode and anodic suppression in anodic electrolyte decomposition.

Poster Presentation : **MAT.P-493**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Enhancing p-type thermoelectric properties of polycrystalline Bi2Te3-based materials via MnTe2 incorporation

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Bi2Te3-based materials have been known for representative thermoelectric material near ambient temperature. However, commercial applications of Bi2Te3-based thermoelectric modules have been limited due to the low performance. The energy conversion efficiency of the modules is evaluated by thermoelectric figure of merit (ZT) over the entire operating temperature region, it is therefore of importance to increase average ZT in the full range of operating temperature. Herein, we report the enhancement of Bi2Te3 thermoelectric system via inclusion of MnTe2. MnTe2 incorporation simultaneously increases both carrier concentration and mobility unlike the general behavior of semiconductors, which results in enhancement of power factor up to ~ 45 μW cm-1 K-2 at 327 K. At the same time, It also significantly decreases lattice thermal conductivity down to ~0.50 W m-1 K-1 at 373 K. Through the synergetic effects, Bi2Te3-MnTe2 system accomplish a remarkably high average ZT of ~1.21 from 300 to 500 K and ZTmax ~ 1.34 at 400 K .

Poster Presentation : **MAT.P-494**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Ge/GeO2/RuO2 nanocomposite as enhanced anode materials for Li ion Batteries

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

Transition metal oxides have been studied as promising electrode materials for lithium ion batteries (LIB) with multiple process of Li ion storage mechanism which can implement high theoretical capacity. However, the low conductivity and poor cyclability caused by volume variation during lithiation/delithiation have been pointed out as a limit that made practical application difficult. We synthesized new anode material (Ge/GeO2/RuO2) with enhanced ionic conductivity and high pseudocapacitance by manufacturing two-dimensional RuO2 nanosheets chemically and hybridizing them with germanium-containing nanoparticles. The CV analysis revealed that the contribution of the capacitive ion storage process to diffusion controlled process was significantly increased in Ge/GeO2/RuO2 compared to the bare Ge/GeO2 nanoparticles (Ge/GeO2 NPs). In addition, charge/discharge test showed that Ge/RuO2 has improved rate capability, and much higher specific capacity and cyclability than Ge/GeO2 NPs and layered RuO2, respectively.

Poster Presentation : **MAT.P-495**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Device Fabrication of Heterostructured TMDCs Formed by Selective Sulfurization Through Graphene Masks

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Transition metal dichalcogenide (TMDC) has been continuously investigated as a variety of semiconducting devices due to its unique optical and electrical properties such as its electron mobility, high on/off ratio, and *etc*. Since one of the obstacles limiting the performance of such devices is contact resistance between channel and electrode, various studies have been introduced to overcome. Among them, the contact geometry plays an important role in contact resistance. The top contact, van der Waals interaction between channel and electrode, induces an additional Schottky barrier, while the edge contact does not induce and does provide higher electron mobility. However, edge contact is difficult to be realized especially for large-scale production in that it requires complex fabrication method such as *in-situ* dry etching.Here, we fabricated van der Waals MoS_2-WS_2 vertical heterostructures as well as MoS_2 and WS_2 single structures with multilayer graphene mask, sulfurizing Mo and W thin film to its sulfide structure. The graphene mask effectively inhibited sulfurization of thin film which played a role of gas barrier, while metal thin film without graphene mask was transformed to metal sulfide by hydrogen sulfide gas. With the proposed selective sulfurization, edge contact between electrode and channel was achieved, exhibiting higher electrical performance than the conventional devices with typical electrical contact.

Poster Presentation : **MAT.P-496**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Blue light-emitting electrochemical cells based on ionic small molecules

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Light-emitting electrochemical cells are the future generation of display and solid state lighting sources.[1]. Compared to conventional solid state lighting device such as organic light-emitting diode (OLED), (LECs) possess simple device architecture and air stable electrodes makes LECs more impressive. Mainly LECs are two types, p-LECS and Ir-ITMCs. Polymer LECs are tri-component blend containing emitting polymer, an ion-conducting polymer and an inorganic salt. Currently much research has been focused on cationic iridium complexes due to the phosphorescent, color tuning and an ionic nature of Ir-ITMCs. Recently non-ionic small molecule light-emitting electrochemical cell containing the device structure as same as the p-LEC were reported by Tang et al.[2]. The molecule which is an ionic apart from Ir-ITMCs have great attentions. We report LECs based on an ionic fluorene derivatives as an active component.References[1] Pei,Q., Yu, G., Zhang, C., Yang, Y., Heeger, A.J., Science, 269, 1086 (1995).[2]Tang, S., Tan, W., Zhu, X., Edman, L., Chem. Commun., 49, 4926-4928 (2013).

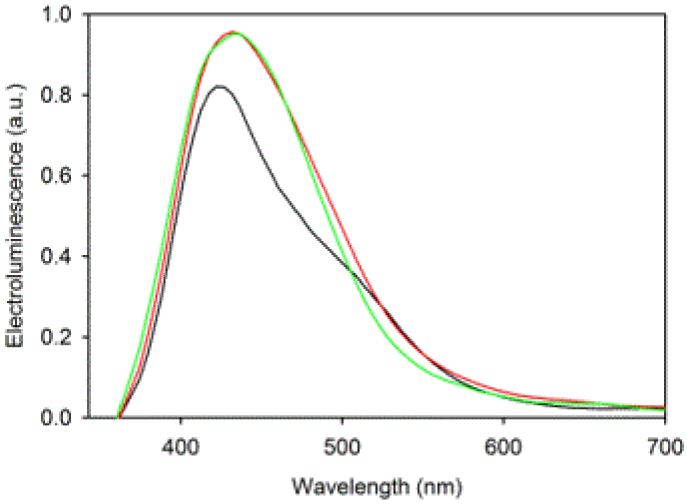

Figure 1: Electroluminescence spectra of active compounds.

Poster Presentation : **MAT.P-497**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Green light-emitting electrochemical cells based on ionic small molecules

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Light-emitting electrochemical cells (LECs) are considered as the next-generation lighting sources as a potential replacement for organic light-emitting diodes (OLEDs). Ionic organic small molecules (SMs) have established the applicability in solid-state lighting, and is seen as a prospective active material for LECs with higher device performance. In this study, we report the design and synthesis of two new green fluorescent light emitting ionic small molecules with triazine acceptor. The synthesized green emitters showed excellent solubility, high luminescence in solution and solid state, high thermal stability, and good film-forming abilities. Thermal stabilities were noted to be very high at 370 and 358 °C for these molecules. The glass transition temperatures were also noted to be very high 120 and 104 °C. These nondoped LEC device exhibited green emission at 505 and 499 nm with Commission Internationale de I'Eclairage coordinates of (0.28, 0.54) and (0.27, 0.52).

Poster Presentation : **MAT.P-498**

Materials Chemistry

Zoom 8 WED 17:30~18:00

Highly selective sucrose detection using carbon nanotube based field effect transistor

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A carbon nanotube decorated with Au nanoparticles (Au-CNTs) could be an active sensing element of a field-effect transistor (FET) for the sensitive detection of sucrose among the sugar family (glucose, fructose and sucrose). The sensor showed high sensitivity for sucrose (0.64 mM^{-1}) up to 2.5 mM, but it showed extremely low sensitivity for glucose (~0.28 mM $^{-1}$) and fructose (~0.05 mM^{-1}). The origin of the selective detection mechanism might be the increased potential barrier between the conductive CNTs by the adsorption of the bulky sucrose on the surface of the attached Au nanoparticles. We demonstrated that the Au-CNT-FET could be a good biosensor for the fast and easy detection of sucrose level among the concentrated sugar mixture in a honey and a sports drink within acceptable error range in food industry, ~1%.

Poster Presentation : **MAT.P-499**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Biomimetic Moth-Eye SiO2 Pattern via Polystyrene Nano-Sphere Lithography for Enhancing Extrusion Efficiency

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In an attempt to improve the efficiency of light extraction, biomimetic moth-eye SiO2 structures were fabricated on ITO-coated glass substrate by a combination of polystyrene (PS)-based nano-sphere lithography (NSL), with a hexagonal-closed-packing array, and reactive ion etching (RIE) using O2 and CHF3 gas. Dimensions of height and diameter of PS nano-sphere can be adjusted by selective gas etching process. Compared to the reflection of flat ITO/glass substrates, the surface reflection of moth-eye patterned ITO/glass decreases with gradual change of refractive index, resulting in an increase in the amount of transmitted light. In addition, by coating MgF2 of 98 nm using electron-beam deposition on ITO layer of substrate, the moth-eye SiO2 pattern was able to minimize optical loss to visible wavelength. The measurement result for our nanostructure, with a diameter and height of 180 nm and 230 nm, respectively, was a 3% reflectance reduction in the 380 ~ 780 nm range compared to the reflectance of a flat ITO/glass substrate. For multi-functional surface modification, we performed self-assembled monolayer (SAMs) treatment by applying perfluorosiloxane (PFS) to the moth-eye nanostructure. A field emission scanning electron microscope (FE-SEM) was used to investigate the morphology of the anti-reflection (AR)-patterned SiO2 nanostructure and hydrophobicity of the nanostructure was measured by contact angle measurement.

Poster Presentation : **MAT.P-500**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Synthesis and instrumental charactericstics of the selected Quinophthalone and Azopyridone derivatives renowned for yellow colorants

Soo-Yeon Yang

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The materials in digital printing ink was used in the range of colorants as a display color filter. In the midst of their yellow colorants, Quinophthalones and Azopyridone derivatives were selected to compared with the existing characteristics.Quinophthalone were synthesized that 2-Methylaminoquinoline and phthalic anhydride reacted at 220 ℃ with catalyst ZnCl2 under N2 gas purging. 2,4-disubstituted phenylazo-pyridone derivatives which have been used for the dyeing of fabrics, were prepared by reacting the diazonium salts of 2,4-disubstituted phenylamines with a l-substituted-2-hydroxy-4-methyl-5-cyano-6-pyridone component. Their spectral chracteristics and thermal property were verified by NMR, IR, UV and TGA analysis.

Poster Presentation : **MAT.P-501**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Facile Synthesis of Narrow-Band $SrMgAl_{10}O_{17}$:Eu,Mn Green Phosphors and Three-Package White LED Backlighting Applications and Photoluminescence Properties

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

$BaMgAl_{10}O_{17}$ (BAM) phosphors, due to the good quality of their blue emission, have long been used for plasma display panels (PDPs). However, because BAM phosphors are excited by harmful vacuum ultraviolet (VUV) light, they are no longer used. For this reason, we substituted cation Ba^{2+} with Sr^{2+} ion using a BAM phosphor and the excitation light was enhanced in addition to the red shift of the excitation spectrum through Eu^{2+} and Mn^{2+} co-doped $SrMgAl_{10}O_{17}$ (SAM) phosphors, allowing the use of a near-blue LED (430 nm). The photoluminescence (PL) emission spectra of SAM:Eu,Mn phosphor peaks at 518 nm at a full-width-at-half-maximum (FWHM) of 26 nm under LED excitation at 430 nm. Using these results, we fabricated three-package down-converted white-LEDs (DC-WLEDs) with a 430 nm blue LED and $K_2SiF_6:Mn^{4+}$ (KSF:Mn) red phosphors. Optimal SAM:Eu,Mn green and KSF:Mn red phosphors have a color-filtered RGB triangular gamut range similar to that of the NTSC standard system in the CIE 1931 color space. The color space has been enlarged by 114%. The luminous efficacy of our DC-WLED was measured and found to exceed 90 lm/W at 20 mA. Hence, it can be confirmed that these phosphors are feasible for use as backlighting components of LCDs.

Poster Presentation : **MAT.P-502**

Materials Chemistry

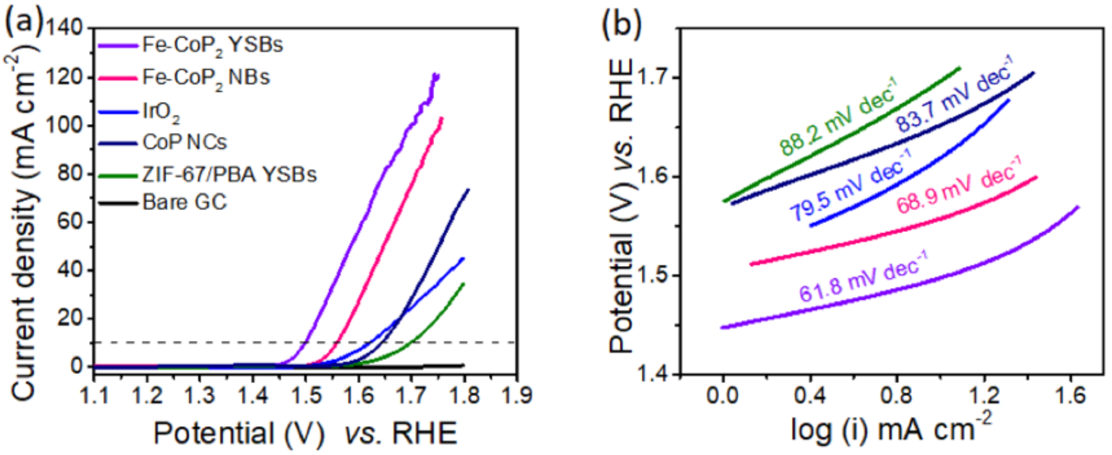
Zoom 8 WED 17:30~18:00

Electrocatalytic properties of CoP_2/Fe-CoP_2 yolk-shell nanoboxes for oxygen evolution reaction

Ganesan Vinoth, Jihye Son, Jinkwon Kim*

Department of Chemistry, Kongju National University, Korea

To achieve comercilization of the effective production of H2 gas through water splitting, efficient electrocatalysts for oxygen evolution reaction (OER) are eccential. In this presentation, we demonstrate rational design and electrocatalytic properties of CoP2/Fe-CoP2 yolk-shell nanoboxes for the OER. Benefiting from the unique hollow structure and chemical composition, the CoP2/Fe-CoP2 YSB electrocatalyst has high specific surface area of 114 m2g-1, and shows superior electrocatalytic performances for OER such as low overpotential of 266 mV, small Tafel slope value of 68.1 mV dec-1, and excellent cyclic stability.



Poster Presentation : **MAT.P-503**

Materials Chemistry

Zoom 8 WED 17:30~18:00

Synthesis of NiP_2 hollow nanostructures using Ni-BDC crystals as structural templates

Jihye Son, Chaeeun Lee, Jinkwon Kim[*]

Department of Chemistry, Kongju National University, Korea

In this presentation, we demonstrate a rational design and synthesis of nickel phosphide hollow nanostructures by etching Ni-BDC crystals and subsequent phosphidation. Uniform tetragonal rod shaped Ni-BDC nanocrystals were obtained by ultrasonication method. Etching Ni-BDC crystals with different amount of water in organic solvents resulted in the formation of various crystal structures such as tetragonal tube and very thin layered structure which were converted to Ni2P by phosphidation in a tube furnace. The products were characterized by XRD, XPS, SEM, TEM, and EDS analysis. Electrochemical properties of these materials will be also discussed.

Poster Presentation : **MAT.P-504**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Investigation on doping dependent optical properties of N-carbon dots

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Carbon dots are emerging new class of nanomaterials with low toxicity, simple and low-cost synthesis process, high biocompatibility, and excellent fluorescent properties. These unique properties of carbonic dots have inspired extensive studies on them due to their great potential for a wide variety of technical applications including cell labeling, therapy, catalysis, energy and storage. Especially, their low toxicity and biocompatibility prompted the creation of CQDs to replace semiconductor quantum dots which possess toxicity issues. In this work, N doped carbon dots were obtained by varying the reaction ratio of citric acid and ethylenediamine. N dependent optical properties of carbon dots were investigated and optimized

Poster Presentation : **MAT.P-505**
Materials Chemistry
Zoom 8 WED 17:30~18:00

Artificial enzyme: N doped carbon dots and their enzymatic properties depending on N degree

Sohee Yun, Jin-sil Choi*

Department of Chemical and Biological Engineering, Hanbat National University, Korea

Nanozymes are nanomaterial-based artificial enzymes which have successfully served as direct surrogates of traditional enzymes for catalysis. Nanozymes offer higher catalytic stability, ease of modification and lower manufacturing cost than protein enzymes. Carbon dots is one of the powverful candidates because of their unique properties as compared to natural enzymes and/or classical artificial enzymes. In this work, we systematically investigated the enzymatic property of carbon dots in which amount of nitrogen is controlled.the peroxidase mimicking properties of a series of carbon dots which was controlled thier N doping degree by varying the ration of reactants.

Poster Presentation : **ELEC.P-506**

Electrochemistry

Zoom 9 WED 16:30~17:00

Fabrication of a Size-gradient Structure of Porous Silicon for a Miniature Spectrometer Application

Byoung-Yong Chang

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Here, we report on an application of bipolar electrochemistry utilizing an interfacial potential gradient that is distributed on a silicon electrode to generate a porous silicon film, which behaves as an optical rugate filter with a stop-band that varies in wavelength across the film surface. While the electrode employed is not bipolar because only oxidation is required to etch the silicon wafer, the fundamental concept of bipolar electrochemistry is exploited to generate the anodic current gradient on the silicon anode. When imaged with a smartphone camera and analyzed with the appropriate image processing algorithm, the gradient filter acts as a rudimentary spectrometer. Test spectra are obtained and benchmarked to a conventional CCD spectrometer.

Poster Presentation : **ELEC.P-507**
Electrochemistry
Zoom 9 WED 16:30~17:00

MnO2 and banana peel derived porous carbon composites for supercapacitors application

<u>Guijun Yang</u>, Soo-Jin Park[1,*]

Department of Chemistry, Inha University, China
[1]*Department of Chemistry, Inha University, Korea*

MnO2/biomass-derived porous carbon (BPC) composites have been prepared by a hydrothermal method, in which the BPC 3D porous carbon structure was based on a banana peel. The banana peel, after freeze drying, can maintain its hierarchical natural porous structure, which provides enough growth space for MnO2 and reduces the agglomeration of MnO2 particles. The MnO2/BPC composites were characterized by XRD, FT-IR, XPS, TGA, SEM, TEM, BET. The electrochemical performance of the composites was tested in three-electrode supercapacitors using 1 M Na2SO4 aqueous solution as an electrolyte. Due to the large amounts of hierarchical pores and large pore volume, the as-prepared composites exhibited good electrochemical performance. Electrochemical measurements indicated that the MnO2/BPC composites applied in supercapacitors had a specific capacitance of 139.6 F g-1 at 300 mA g-1, and exhibited a good cycling stability with a capacitance retention ratio of 92.3% after 1000 cycles (at 1 A g-1). The MnO2/BPC composites with 3D porous structure are promising materials in the application of supercapacitors.

Poster Presentation : **ELEC.P-508**
Electrochemistry
Zoom 9 WED 16:30~17:00

Synthesis of Li4Ti5O12 anode materials with high specific capacity for lithium-ion batteries

Guijun Yang, **Soo-Jin Park**[1,*]

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

We prepared Li4Ti5O12-y solid solutions by one-step solid-state carbon thermal reduction reaction. Samples of Li4Ti5O12-y solid solutions are synthesized with different content of carbon black. The presence of carbon black act as reductant. The formation mechanism of Li4Ti5O12 in the presence of carbon (carbon black) was investigated. Moreover, the effect of Ti3+ on the electrochemical performance of the Li4Ti5O12-y solid solutions has been investigated systematically. Among all samples, the sample with 2% carbon black additive exhibited the highest discharge capacity and best cycling stability. Our findings reveal that the surface modification with carbon black can improve the electrical conductivity and Li+ diffusion coefficient and improve rate capacity and cycling stability significantly.

Poster Presentation : **ELEC.P-509**

Electrochemistry

Zoom 9 WED 16:30~17:00

Synthesis of carbon-based NiCo2O4 as electrodes for an asymmetric supercapacitors

Guijun Yang, **Soo-Jin Park**[1,*]

Department of Chemistry, Inha University, China
[1]*Department of Chemistry, Inha University, Korea*

We demonstrate a simple hydrothermal approach to obtain a carbon-based NiCo2O4 material for use in supercapacitors. In this process, filter paper was submerged in a NiCo2O4 precursor solution, and the final product was obtained after calcination in an Ar2 atmosphere. The hydroxyl group-containing cellulose in the filter paper facilitates the formation of 3D structures, which not only improve the electrical conductivity but also provide fast electron and ion transport after calcination at high temperature, thus improving the electrochemical performance. An asymmetric supercapacitor has been assembled by using NCO/C-2 and activated carbon as the positive and negative electrodes. The NCO/C-2//AC ASC device exhibits a maximum energy density of 20.87 Wh kg-1 at a power density of 374.6 W kg-1 and a maximum power density of 7.48 kW kg-1 at an energy density of 11.43 Wh kg-1.

Poster Presentation : **ELEC.P-510**

Electrochemistry

Zoom 9 WED 16:30~17:00

Role of Electrical Field for Transformation of Perovskite Quantum Dots Tracking through *In-situ* Spectroelectrochemical Tools

ChaeHyun Lee, KyoungSoo Kim[1], YeJi Shin, Donghoon Han[1,*], Seog Joon Yoon[*]

Department of Chemistry, Yeungnam University, Korea

[1]*Department of Chemistry, The Catholic University of Korea, Korea*

All-inorganic lead halide perovskite quantum dots ($CsPbX_3$, X: Cl, Br, or I, abbreviated as PQDs) operate successfully in various optoelectronic devices, such as solar cells, LEDs, photocatalysis, lasing, and so on. In the devices, the PQDs work under electrochemical bias and/or illumination with charge separation/collection by interacting with charge transport medium. To investigate photoinduced charge transport or charge injection via applied bias, it is inevitable to consider the effects both electrochemical and photochemical environmental condition simultaneously. In-situ spectroelectrochemical tool provides quantitative insights about the spectroelectrochemical behaviors of the $CsPbBr_3$ and $CsPbI_3$ PQDs. We found that the PQDs did irreversible transformation to precursor state of plumbate complexes under electrochemical reaction control. Beyond the certain applied bias, we were able to monitor that hole mediate electrochemical oxidation of the PQD impacts the irreversible transformation. Understanding such charge transfer mediated process could provide the way to develop practical strategy for utilization of the PQDs to optoelectronic devices.

Poster Presentation : **ELEC.P-511**

Electrochemistry

Zoom 9 WED 16:30~17:00

Ultra Compact Nanoporous Platinum Coating Improves Neural Recording

Je Hyun Bae, Taek dong Chung[1,*]

Graduate School of Analytical Science and Technology, Chungnam National University, Korea
[1]*Department of Chemistry, Seoul National University, Korea*

Neural electrodes are key tools for achieving a successful brain-computer interface (BCI) and the electrodes should be small to minimize damage to neural tissue and obtain good spatial selectivity such as single unit recording. For this, the key strategy is to develop a material that can significantly lower the electrode impedance without changing the apparent area before and after modification of bare electrodes. Here it is shown that conventional platinum/tungsten neural probes can be coated with nanoporous Pt using electrochemical depositions. Thanks to nanoporous Pt with the extremely small (1-2 nm) and uniform pores, L_2-ePt, the electrode impedance could be reduced by more than 3 orders of magnitude while the apparent area was almost the same. L_2-ePt coating enhanced neuronal recording of local field potential in monkeys, leading to facilitating implanted electrical devices in the nervous system.

Poster Presentation : **ELEC.P-512**
Electrochemistry
Zoom 9 WED 16:30~17:00

Flake size and porosity effects of activated graphene on the performance of silicon/activated graphene composites as lithium-ion battery anodes

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Program in Nano Science & Technology, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, Republic of Korea, Korea

Activated graphene (AG) has been receiving much attention for energy storage application as its in-plane holes in basal planes can facilitate abundant active surface areas and shortened ion diffusion pathways. Exposing graphene to acid solution is common method to generate in-plane pores into the graphene sheets. Although introduction of defects into the graphene cannot avoid graphene sheet breakage, little attention has been paid to flake size of the AG. Therefore, the control of the defects needs to be clarified together with the investigation of the flake size on electrochemical properties of the AG. To unveil influence of both the flake size and porosity, a series of AG was synthesized with different acid treatment time and the resulting AGs are composited with silicon nanoparticles (SiNPs). A series of silicon/reduced activated graphene (Si/rAG) composites are electrochemically tested as anode materials for lithium-ion batteries. In terms of electrochemical performance, Si/rAG-4h electrode exhibits the best rate and cycle performance among the Si/rAG samples due to its optimal properties of AG-4h. Increasing acid etching time for the AG synthesis results that in-plane pore size bigger, along with facile lithium-ion diffusivity, while the AG flakes undergo breakage that can trigger decreased electrical conductivity. Herein, the trade-off relationship between the lithium-ion diffusivity and the electrical conductivity on the electrochemical performance has been well studied. This investigation is helpful for design AG-based composites for high-performance electrochemical devices considering both the flake size and the porosity in AG synthesis.

Poster Presentation : **ELEC.P-513**
Electrochemistry
Zoom 9 WED 16:30~17:00

An Oligonucleotide-based Electrochemical Sensor for Sensitive and Selective Detection of Silver(I)

Kyoungsoo Kim, Je Hyun Bae[1], Donghoon Han*

Department of Chemistry, The Catholic University of Korea, Korea
[1]*Graduate School of Analytical Science and Technolo, Chungnam National University, Korea*

We have developed a sensitive and selective electrochemical sensor for the detection of silver(I) ions in aqueous media. This electrochemical sensor is based on the molecular beacon which involves an electroactive, methylene blue-labeled DNA hairpin structure and provides selective binding of cytosine-cytosine mismatch for Ag^+ ions. The methylene blue-labeled DNA as self-assembled through S-Au bonding on a gold electrode surface and the surface blocked with 6-mercapto-1-hexanol to form a mixed monolayer. The modified electrode showed a electrochemical signal due to a redox reaction which changes methylene blue to leucomethylene blue. The “signal-on” upon silver binding could be attributed to change in conformation from open structure to restricted hairpin structure. The DPV of modified electrode showed a linear response of the methylene blue reduction signal with increase of Ag^+ concentration in the range between 10 nM and 500 nM. The molecular beacon silver(I) ion sensor was regenerated by unfolding the methylene blue-labeled DNA in 0.1 M EDTA solution.

Poster Presentation : **ELEC.P-514**

Electrochemistry

Zoom 9 WED 16:30~17:00

Supercapacitive behaviors of activated carbons derived from coffee grounds

Ui-Won Lee, Soo-Jin Park*

Department of Chemistry, Inha University, Korea

In this work, activated carbon prepared from waste coffee grounds using chemical activation. Activated microporous carbons were synthesized from coffee grounds by a one-step synthesis. The activated microporous carbon materials obtained from wasted coffee grounds prepared at various ratio KOH. Activated carbon materials prepared using KOH have a strong potential for application in supercapacitor electrodes due to their specific surface area and narrow micro pore distribution. The pore properties of porous materials are evaluated by inert gas adsorption (in N_2 at 77 K). Additionally, cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) tests were employed in the evaluation of the electrochemical behavior of each sample. From the result, it was found that the creation of microporosity introduced by KOH affected in specific capacitance. This work highlights the potential to utilize waste coffee grounds to produce electrode material for energy storage systems.

Poster Presentation : **ELEC.P-515**

Electrochemistry

Zoom 9 WED 16:30~17:00

Electrochromic properties of mixed Iron/Nickel hexacyanoferrate(III) thin films

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Prussian blue(PB) is a well-known electrochromic material with a polyelectrochromic property and four redox states: the colorless Prussian white(PW), PB, Berlin green (BG), and Prussian yellow (PY), in sequence from most reduced to the most oxidized state. Because PB ⇔ PW redox reaction is much more stable than PB ⇔ PY reaction, it is applied to electrochromic devices. However, consumers' low preference for blue requires color modulation.In this study, we syntehsized mixed iron/nickel hexacyanoferrate (Fe-Ni-PBA) nanoparticles for color modulation and characterzed by XRD, SEM, EDS, UV-Vis spectrometer and cyclic voltammetry.Fe-Ni-PBA thin films were prepared by sol-gel coating on flexible PET/ITO substrate. As the Nickel content increased, the maximum absorbance of the thin films shifted from 680 nm to 750 nm, and showed excellent durability not only in PB ⇔ PW redox reactions but also in PB ⇔ PY redox reactions.

Poster Presentation : **ELEC.P-516**
Electrochemistry
Zoom 9 WED 16:30~17:00

Preparation and characterization of rice husks based activated carbon for improving specific capacitance

Ui-Won Lee, Soo-Jin Park[*]

Department of Chemistry, Inha University, Korea

In this work, activated carbon (AC) prepared from rice husk using chemical activation. ACs were treated with various activation temperatures. Activated carbon materials prepared using KOH have a strong potential for application in supercapacitor electrodes due to their specific surface area and narrow micro pore distribution. Therefore, appropriate control over pore size distributions is a key factor for good electrochemical performance. The porosity and surface structure of ACs are highly dependent on the activation temperature. Examination of the morphology of the prepared samples by scanning electron microscopy (SEM). The electrochemical performance of the prepared materials was characterized by cyclic voltammetry (CV) and galvanostatic charge/discharge (GCD) measurements using an IviumStat electrochemical workstation. This work highlights the potential to utilize rice husks to produce electrode material for energy storage systems.charge/discharge (GCD) measurements using an IviumStat electrochemical workstation.

Poster Presentation : **ELEC.P-517**

Electrochemistry

Zoom 9 WED 16:30~17:00

Electrochemical performance of the mixed solid electrolyte (100-x)Li3SI-xLi6PS5Cl(x=0, 5, 10, 15 and20) for all solid state lithium batteries

Minho Park, Kwang Sun Ryu*

Department of Chemistry, University of Ulsan, Korea

Li_3OX (X=Cl, Br, and I) called lithium rich anti-perovskite materials recently reported as super ionic conductors with 3-dimensional Li migrating channels. Li_3OX with anti-perovskite structure as solid electrolytes exhibits thermodynamic stability. These materials have low melting point and high electrochemical stability. But Li_3OX phase tends to decompose into more stable LiX and Li_2O phases at service temperature of interest for LIBs. As the Li_2O phase is a rather poor ionic conductor, it would be useful in examining the feasibility in substitution of O by other chalcogen elements such as S. To prevent the decomposition of the substance, Li_3OX(X=Cl, Br, and I) anti-perovskite was synthesized by replacing S with O. The Li_6 PS_5Cl argyrodite solid electrolyte is known as solid electrolyte with high ionic conductivity of 10^{-2}~10^{-4}S/cm at room temperature. Moreover, the high ionic conductivity could be achieved by optimizing the mechanical milling and the annealing processes. However, there is a disadvantage in that electrochemical stability is so lower than Li_3SI. Based on above studies, we have synthesize (100-x)Li_3SI-xLi_6 PS_5Cl (x=0, 5, 10, 15, 20) to increase the lithium ionic conductivity and electrochemical stability of them. We analyzed the crystal structures of them by XRD. As the electrochemical analysis, electrochemical impedance spectroscopy with various temperatures was conducted to evaluate Li+ conductivity of the materials. Further, the electrochemical performance such as cyclic voltammetry, DC-cycling, and charge and discharge tests were conducted to make synergic effects.

Poster Presentation : **ELEC.P-518**
Electrochemistry
Zoom 9 WED 16:30~17:00

Trimetallic double hydroxide nanosheets derived from graphene oxide for enhanced oxygen evolution reaction

Jihyun Kim, Sunguk Noh, Jun Ho Shim[*]

Department of Chemistry, Daegu University, Korea

Layered double hydroxides (LDHs) are a typical class of layered materials with a general formula of [(MII)1-x(MIII)x(OH)2]x+(Am-x/m)·nH2O] and are one of the most promising technical methodology for oxygen evolution reaction (OER) because of their low cost, ease of preparation, and the large number of composition. Negative charged graphene oxide (GO) was found to be more beneficial for LDHs outgrowth and branching because metal ions are positively charged. We report a very simple and efficient approach to the preparation of GO encapsulated NiCoFe-LDH nanocomposites via a hydrothermal method. The trimetallic LDH nanosheets exhibit high catalytic activity towards OER. Moreover, these trimetallic LDHs exhibit excellent stability in alkaline electrolytes. For comparison, other double-combination LDHs were also studied. The compositional/structural features are characterized by scanning electron Microscope, high-resolution transmission electron microscopy, X-ray photoelectron spectroscope, and X-ray diffraction. We also investigate the electrocatalytic activity of rGO/NiCoFe-LDH for OER in alkaline media by rotating disk electrode, rotating ring-disk electrode, and cyclic voltammetry. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : **ELEC.P-519**

Electrochemistry

Zoom 9 WED 16:30~17:00

Trimetallic Co-M-Fe (M = Ni, Mn, Cu) catalysts for low overpotential water splitting

Sujin Jo, Jun Ho Shim*

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Research on energy conversion using renewable energy sources has long been considered a promising strategy for improving the performance of electrochemical cells. Non-precious metallic nanocomposites are technologically promising for renewable energy storage and conversion. In this presentation, a series of trimetallic nanocomposites (Co-M-Fe; M = Ni, Mn, Cu) were fabricated from a Prussian blue analogue (PBA) strategy. The resulting Co-M-Fe materials were calcined at 300 ℃ to obtain the final products. The oxygen evolution reaction (OER) catalytic performance of the Co-M-Fe catalytic series and commercial Ir/C benchmark catalysts was investigated using a rotating-disk electrode (RDE) under alkaline conditions. The Co-Ni-Fe composite was superior to the Co-Mn-Fe, Co-Cu-Fe, and Ir/C catalysts. Enhanced OER activity was determined further by stability testing in a 1.0 M KOH solution. The compositional/structural features are characterized by high-resolution transmission electron microscopy, Brunauer-Emmett-Teller analysis, X-ray photoelectron spectroscopy, and X-ray diffraction. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : **ELEC.P-520**
Electrochemistry
Zoom 9 WED 17:00~17:30

Ca-doped CuS Counter Electrodes for High Efficiency Quantum Dot Sensitized Solar Cells

Mohammed Panthakkal abdul muthalif, Youngson Choe[1,*]

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The present study reports the incorporation of calcium (Ca) into the CuS counter electrodes (CEs) in order to modify the photovoltaic performance of quantum dot-sensitized solar cells (QDSSCs). Ca-doped CuS CEs were prepared by the chemical bath deposition (CBD) method on FTO substrate. For the Ca-doped CuS thin films, copper nitrate and thioacetamide were used as cationic and anionic precursors. Calcium nitrate tetrahydrate was used as doping material. The changes observed in the diffraction patterns suggest that Ca dopant can introduce increased disorder into CuS material structure. EDX analysis was employed to determine the elemental identification and the results confirmed the presence of Cu, S, and Ca on the FTO glass substrate. Electro chemical impedance spectroscopy results displays that Ca-doped CuS CEs have greater electrocatalytic activity and charge transport capacity than that of bare CuS. Photovoltaic performance studies demonstrate that 20% Ca-doped CuS CE based QDSSCs exhibit superior power conversion efficiency (η) of 4.92%, short circuit current density of 15.47 mA cm-2, open-circuit photovoltage of 0.611 V, and fill factor (FF) of 0.521 under illumination of one sun.

Poster Presentation : **ELEC.P-521**

Electrochemistry

Zoom 9 WED 17:00~17:30

Spherical FeOF Nanoparticles Wrapped in Graphitic Carbon Derived from Maleopimaric Acid as a Cathode Material for Sodium-Ion Batteries

Achmad Yanuar Maulana, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Sodium-ion batteries (SIBs) are considered one of the most promising energy storage systems for replacing lithium-ion batteries because of the high abundance and low cost of sodium. Iron oxyfluoride (FeOF) is a promising conversion-based cathode material for SIBs because of its high theoretical capacity of about 855 mAh g^{-1} and low-cost chemical compositions and its lower sensitivity to the size of charged carrier ions. However, the poor electrical conductivity and ion diffusion of FeOF result in a low rate capability and cyclability. In this work, FeOF nanoparticles wrapped by graphitic carbon layers were synthesized using abietic or maleopimaric acid as both the carbon source and organic ligand. In addition, the morphology of the FeOF particles was gradually controlled from rod to spherical shapes, simply depending on the rosin acids. The FeOF nanoparticles prepared with maleopimaric acid showed a large reversible discharge capacity of 356.7 mAh g^{-1} with a fading rate of 0.21% per cycle after 100 cycles at a current density of 100 mA g^{-1} and an excellent rate capability as a cathode for SIBs.

Poster Presentation : **ELEC.P-522**

Electrochemistry

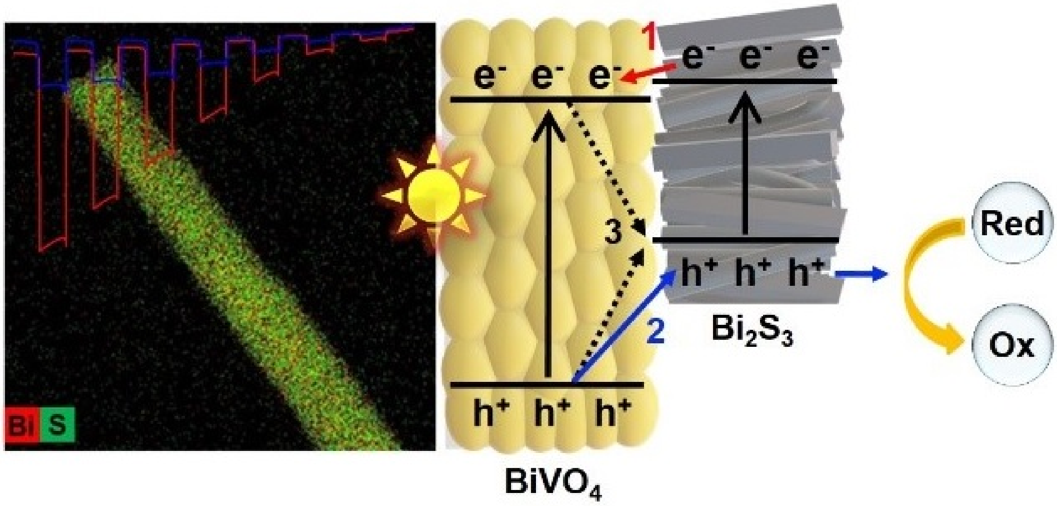
Zoom 9 WED 17:00~17:30

Understanding of growth mechanism and photoelectrochemical activity of $BiVO_4/Bi_2S_3$ nanowire composite

Changhyun Hong, **Ki Min Nam***

Department of Chemistry, Pusan National University, Korea

A $BiVO_4/Bi_2S_3$ composite comprising Bi_2S_3 nanowires on top of $BiVO_4$ film was prepared via hydrothermal process. As additional Bi^{3+} ions were not provided during the reaction, the $BiVO_4$ served as the Bi^{3+} source for the growth of Bi_2S_3. Detailed growth mechanism of the nanowire was elucidated by an analysis of the concentration gradient of Bi^{3+} and S^{2-} ions during the reaction. The in situ growth was followed by the etching of $BiVO_4$ to Bi^{3+} and VO_4^{3-} ions and regrowth to Bi_2S_3, which resulted in the rapid development of nanowires on the $BiVO_4$ substrate. The fabricated $BiVO_4/Bi_2S_3$NW composite exhibited an improved photoelectrochemical activity compared to other Bi_2S_3 samples. The improved efficiency was mainly attributed to both improved charge separation and effective adhesion obtained by the in situ growth.



Poster Presentation : **ELEC.P-523**
Electrochemistry
Zoom 9 WED 17:00~17:30

A Constant Phase Element at Nanoporous Electrodes

Je Hyun Bae

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

A constant phase element (CPE) is an equivalent electrical circuit component that models the behavior of a double layer, which is a kind of imperfect capacitors. In general, it is known that the exponent α at CPE depends on surface roughness, surface distribution of capacitance, and adsorbed ions. Nanoporous electrodes have been attracting much attention for diverse applications such as energy conversion devices and sensors. When CPE concept is applied to model the behavior of the electrical double layer at nanoporous electrodes, it is sensitively subject to the roughness, pore shape, and dimension of the nanopores. In this presentation, it is shown that mass transfer along the nanopores affects the CPE, which is significantly different from that of flat electrodes.

Poster Presentation : **ELEC.P-524**

Electrochemistry

Zoom 9 WED 17:00~17:30

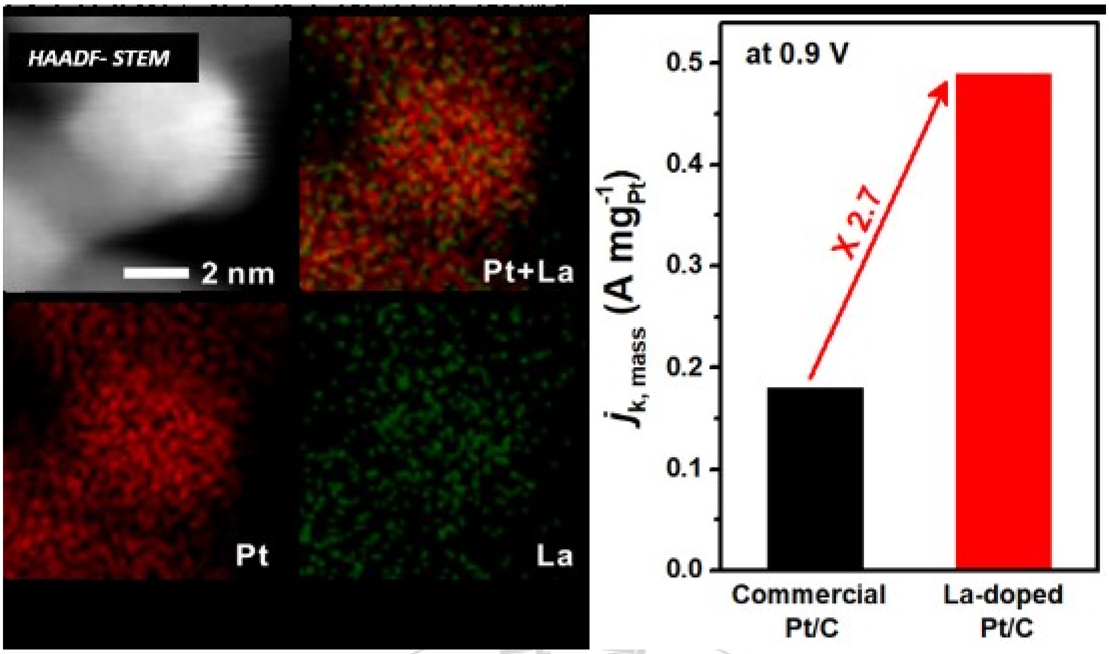
Synthesis and Characterization of La-doped Pt/C nanocatalysts and Their Application towards the Oxygen Reduction Reaction

Jeonghyeon Kim, **Sang-Il Choi**[1,*]

Chemistry, Kyungpook National University, Korea

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

Oxygen reduction reaction (ORR) is a reaction which is the rate-determining step that occurs at the cathode in the proton electrolyte membrane fuel cell. Although Pt-based catalyst have shown great potential as electrocatalysts toward the ORR but the high price of Pt and the limit of resources, and its sluggish ORR kinetics have been the main obstacles. Typical strategy, including formation of alloys with other metals (Ni, Co, Sc, La, and Gd) and doping of transition metals (Mo, Ga, W) on the Pt-based nanocrystal have been investigated to enhance the performance of Pt-based catalysts and thus reduce the use of Pt. Among them, Pt5La alloy showed superior stability after 10,000 times of electrochemical cycles with high ORR mass activity. However, owing to the extremely low reduction potential of La (-2.38 V for La^{3+}/La), it has a difficulty to synthesize and commercialize PtLa catalysts. This presentation reports the new synthesis method to dope La atoms on Pt nanocrystal using molten reducing agent (super-hydride) and simple solvothermal method as a way to improve ORR performance. As synthesized La-doped Pt/C catalysts was confirmed that La doped on the surface of Pt nanocrystal by various techniques, including X-ray diffraction, X-ray photoelectron spectroscopy, X-ray absorption spectroscopy, and energy-dispersive X-ray spectroscopy mapping. The ORR measurement also presented, showing 2.7 times higher mass activity than commercial Pt/C, and just 5.7% reduced performance after 5,000 ORR tests.


HAADF- STEM
2 nm
Pt+La
Pt
La
at 0.9 V
X 2.7
$j_{k,\,mass}$ (A mg_{Pt}^{-1})
0.0
0.1
0.2
0.3
0.4
0.5
Commercial Pt/C
La-doped Pt/C

Poster Presentation : **ELEC.P-525**

Electrochemistry

Zoom 9 WED 17:00~17:30

Facile synthesis of iron-doped porous nickel pyrophosphate nanoparticles for high performance OER electrocatalyst and supercapacitor

Jeongmin Kang, Yuanzhe Piao*

Graduate School of Convergence Science and Technol, Seoul National University, Korea

Recently, transition metal-phosphates have attracted much attention for energy conversion application and electrochemical energy storage. However, the synthesis of such materials generally requires high energy consumption and toxic precursors. In this study, iron-doped porous nickel pyrophosphate (NFPy) nanoparticles were prepared via simple stirring without any heat treatment using the precursor for Ni, Fe, and pyrophosphate. The usage of pyrophosphate promotes the facile Ni oxidation and high chemical stability, overall beneficial to electrochemical applications and environment. The oxygen evolution reaction (OER) performance of NFPy exhibits excellent results that only required the overpotential of 0.210 V to reach 10 mA·cm^{-2}. When used as electrode material for supercapacitor, the NFPy-CNT nanocomposite exhibited a high capacity of 517 C·g-1 at 1 A·g^{-1}.

Poster Presentation : **ELEC.P-526**

Electrochemistry

Zoom 9 WED 17:00~17:30

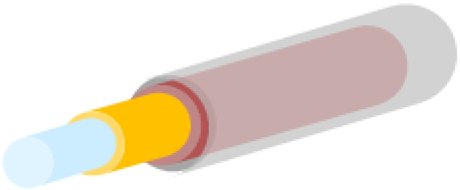
Preparation of TEMPOL Derivatives : Tempol-Adsorbed Li-TFSI Film for Fiber-Shaped Dye-Sensitized Solar Cell.

Myeonghwan Shin, **Chuljin Ahn**[1,*]

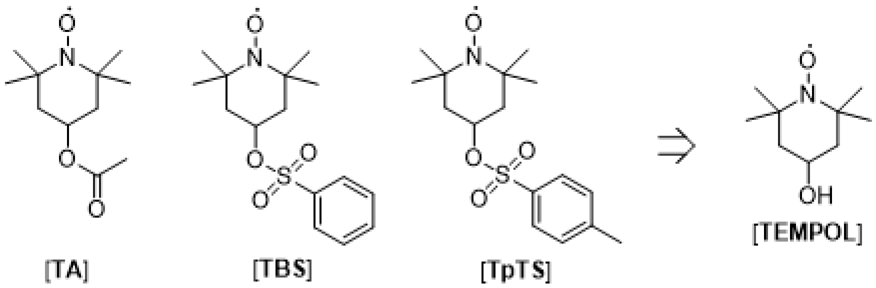
Department of biology and chemistry, Changwon National University, Korea

[1]*Department of Biology and Chemistry, Changwon National University, Korea*

Fiber-shaped solar cells (FSCs) have attracted academically and industrially intense interest due to their light weight, flexibility, weavability, and wearability. FS-DSSC using Li-TFSI film as a quasi-solid-state electrolyte with both traditional electrolyte and TEMPOL electrolyte were first designed. The TEMPOL derivertives as electrolyte were prepared conveniently.



HSE + Li-TFSI film
- HSE Dipping
- Li-TFSI film wrapping
- Dipping of TA, TBS, TMS, and TpTS
- HSE dipping



Poster Presentation : **ELEC.P-527**
Electrochemistry
Zoom 9 WED 17:00~17:30

Synthesis of Crumpled MoS2/N-Doped Carbon Nanosheets as Anode materials for Lithium-ion Batteries

Keunho Lee, **Yuanzhe Piao**[1,*]

Graduate School of Convergence Science and Technology, Seoul National University, Seoul National University, Korea
[1]*Graduate School of Convergence Science and Technol, Seoul National University, Korea*

High-performance anode materials for lithium ion batteries are required due to their increased applications in portable electronic devices and electronic vehicles. In this work, crumpled MoS2/N-doped carbon nanocomposites were synthesized via a simple solventless method. The nanocomposites were identified as homogenously distributed MoS2 in N-doped carbon matrix. The nanocomposites provide the morphological advantages of 3D interconnected electron pathways and an enlarged ionic contact area for improving electrochemical performance when they were used as anodes for lithium ion batteries. Furthermore, the N-doped carbon matrix could enhance electrical conductivity as well as suppressing volume changes during cycling. The nanocomposites demonstrated a reversible discharge capacity of 264 mAh g-1 at 10 A g-1 and a stable cycle life with a discharge capacity of 324.2 mAh g-1 and coulombic efficiency of 99.7%, even after the 1000th cycle at 4 A g-1. These results indicate that the nanocomposites offer great potential as anode materials for lithium ion batteries.

Poster Presentation : **ELEC.P-528**
Electrochemistry
Zoom 9 WED 17:00~17:30

Nanoelectrode as a light guide for photoelectrochemical imaging

Je Hyun Bae, Michael V. Mirkin[1,*]

Graduate School of Analytical Science and Technology, Chungnam National University, Korea
[1]*Department of Chemistry and Biochemistry, Queens College, United States*

Scanning electrochemical microscopy (SECM) has previously been employed in probing photoelectrochemical processes at semiconductor surfaces. However, the spatial resolution of these studies has not yet matched the nanoscale SECM resolution attained without substrate illumination. Herein we introduce nanoscale photo-SECM with a glass-sealed, polished tip simultaneously serving as a nanoelectrode and a light guide to produce a microscopic light spot on the substrate surface. The advantages of this approach are demonstrated by comparing current transients obtained using through-tip and global illumination of the sample. The spot of light on the substrate surface facing the nanotip was sufficiently bright to measure the diffusion-controlled positive feedback current in good agreement with the theory. We employed this approach for high-resolution photoelectrochemical mapping of ferrocenemethanol oxidation and oxygen evolution reactions at the Nb:TiO_2 rutile (110) single crystal surface. The images obtained using 40-50 nm radius tips showed only minor and random variations in photoelectrochemical reactivity for both processes, pointing to essentially uniform distribution of the Nb dopant over the TiO_2 surface and no measurable segregation on the ~50 nm scale.

Poster Presentation : **ELEC.P-529**

Electrochemistry

Zoom 9 WED 17:00~17:30

Surface Charge Effects on Electron-Transfer in Chemically Not Modified Single Carbon Nanopore

Je Hyun Bae, Michael V. Mirkin[1,*]

Graduate School of Analytical Science and Technology, Chungnam National University, Korea
[1]*Department of Chemistry and Biochemistry, Queens College, United States*

Ion transport controlled by electrostatic interactions is an important phenomenon in biological and artificial membranes, channels, and nanopores. Here, we employ carbon-coated nanopipettes (CNPs) for studying permselective electrochemistry in a conductive nanopore. A significant accumulation (up to ~2000-fold) of cationic redox species and anion depletion inside a CNP by diffuse layer and surface charge effects in solution of low ionic strength were observed as well as the shift of the voltammetric mid-peak potential. Finite-element simulations of electrostatic effects on CNP voltammograms show permselective ion transport in a single conducting nanopore and semi-quantitatively explain our experimental data. The reported results are potentially useful for improving sensitivity and selectivity of CNP sensors for ionic analytes.

Poster Presentation : **ELEC.P-530**
Electrochemistry
Zoom 9 WED 17:00~17:30

Integrating Heteromixtured Cu2O/CuO Photocathode Interface through a Hydrogen Treatment for Photoelectrochemical Hydrogen Evoluation Reaction

Young Jun Seo, Soon Hyung Kang[1,*]

Department of Chemistry Education, Chonnam National University, Korea
[1]*Department of Chemical Education, Chonnam National University, Korea*

Cu2O and CuO is a potential semiconductor photocathode with the demonstrated hydrogen production capability. In this work, CuO nanowires were formed on Cu foil substrate by the electrochemical anodization process by immersing them into the alkaline solution under constant current. Despite of the numerous attempts to develop copper oxide heterojunctions via a bottom-up approach, the resulting composites have been suffered from the poor interfacial modulation. However, the intimate modulation through the different ambient annealing of photocathodes could alter the nanostructure, light harvesting, and optical bandgap. Herein, the Cu transforms to Cu(OH)2 by the electrochemical anodization, subsequently transformed to CuO rich Cu2O/CuO composite in air-annealing process. In addition, for the surface engineering of CuO phases, the post-annealing process under the 4% hydrogen-argon mixed gas at 300 °C was performed. As a result, a mild hydrogen treatment (1 min) was found to be effective in enhancing the PEC properties due to the favorable Cu2O/CuO/Cu2O formation, promoting the photogenerated charge separation, the generation of the sufficient cation vacancies closely relating to the electronic conductivity, and the charge-transfer yield. From the XRD and XPS results, it was confirmed that the area of Cu2O has increased by the hydrogen treatment, proving that a slightly thin Cu2O layer was produced from the inherent reduction of prominent CuO phase to modulate as Cu2O/CuO/Cu2O. Overall, the Cu2O/CuO/Cu2O (H2@1min) film exhibited an obvious improvement in photocurrent density of -2.3 mA/cm2 at 0 V vs. reversible hydrogen electrode (RHE)(briefly abbreviated as 0 VRHE) than those nanowires having -1.72 mA/cm2 and -1.44 mA/cm2 of both Cu2O/CuO/Cu (H2@3min) and Cu2O/CuO (Air).

Poster Presentation : **ELEC.P-531**

Electrochemistry

Zoom 9 WED 17:00~17:30

Homocysteine detection using multienzyme co-immobilized electrode

Jeon Sang hyeon, Ik-Soo Shin[1,*]

Chemistry, Soongsil University, Korea
[1]*Information Communication, Materials, Korea*

Hyperhomocysteinemia is a medical condition characterized by an abnormally high level (>15 μmol/L) of homocysteine in the blood, causing complications such as heart attack and arteriosclerosis. Various methods such as high-performance chromatography, gas chromatography, electrophoresis, and electrochemical biosensors have been studied to detect homocysteine. but most of them have a disadvantage in that the operating cost of the device is high and the analysis time is relatively long. In this study, we report a method of electrochemical determination of homocysteine through cascade metabolic reactions of several enzymes. Currently, d-Methionine, an intermediate product of hydrogen peroxide and Cascade reaction, was detected in the range of 15 μmol / L to 200 μmol / L, and linearity exceeding $R^2 = 0.97$ was confirmed.

Poster Presentation : **ELEC.P-532**

Electrochemistry

Zoom 9 WED 17:00~17:30

Increased Brightness and Efficiency of Light-emitting Electrochemical using Host-guest System

Do-hyeong Lee, Ik-Soo Shin[1,*]

Chemistry, Soongsil University, Korea
[1]*Information Communication, Materials, Korea*

Electrochemiluminescence (ECL) is a phenomenon in which light is emitted by an reduction reaction in electrochemical system and, the light-emitting electrochemical cell (LEC) includes the solid-state electrochemical system composed of electrolyte and mobile luminophore and two metal electrode. LECs have various advantages over conventional organic light-emitting diodes such as less independence on the work function of the electrode and the thickness of the emitting layer, low cost fabrication, and versatility in device configuration. Although LEC has these advantages, it is not widely studied yet because of low luminance and poor device life-time. In this study, we demonstrate that the host-guest system, which is a method used in OLED, can be successfully applied to LEC to increase the brightness and external quantum efficiency of the device. Also, the luminance and external quantum efficiency were improved by controlling the ratio of the host and the guest, the concentration of the electrolyte, and the deposition of LiF.

Poster Presentation : **ELEC.P-533**
Electrochemistry
Zoom 9 WED 17:00~17:30

Surface engineering of GaN for efficient water oxidation.

Maheswari Arunachalam, **Soon Hyung Kang**[1,*]

Department of Chemistry, Chonnam National University, Korea
[1]*Department of Chemical Education, Chonnam National University, Korea*

We studied the performance of oxygen (O2) evolution using GaN as photoelectrode in the photoelectrochemical water-splitting system. One of the limitations of nitrides is the decomposition that occurs when the photoelectrode is used at the semiconductor liquid junction. To overcome these limitations, in the present study, we removed the adverse effect of the surface barrier by obtaining the surface inertness of the oxide layer. On the photoanode surface, a native oxide layer with a thickness of a few nm is formed, giving a relatively high efficiency without using any co-catalyst system. The amperometric stability curve obtained for more than 6 hours create a constant photoelectrode performance under illumination (100mW/cm2) using in the alkaline electrolyte.

Poster Presentation : **EDU.P-534**
Chemistry Education
Zoom 10 WED 16:30~17:00

The Effect of the Explanatory Method of Process Viewpoint on Scientific Concept Learning

Sungki Kim, Seounghey Paik[1,*]

Korea Institute for Curriculum and Evaluation, Korea
[1]*Department of Chemical Education, Korea National University of Education, Korea*

According to Chi, most of the scientific concepts belong to a process viewpoint. However, the concepts of process viewpoint consider two or more interactions at the same time, so the learning burden is greater than the concepts of matter viewpoint which consider only one object. Therefore, students tend to consider the concepts of process viewpoint as matter viewpoint. When learning the scientific concepts, learning with wrong viewpoint leads misunderstanding of scientific concept. Nevertheless, textbooks tend not to focus on the viewpoints. Therefore, this study examined the effect of students' scientific concept learning when the explanatory method of process viewpoint for floating and sinking phenomena explicitly is introduced. To this end, we investigated the effect on 44 students in the second year of middle school. As a result of the study, it was found that learning level about scientific concept has risen. Therefore, we would like to propose the introduction of an explanatory method with an explicit process viewpoint.

Poster Presentation : **EDU.P-535**
Chemistry Education
Zoom 10 WED 16:30~17:00

Story about Education and Life Reflected in the Overseas Voluntary Activity of Science Education

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Department of Chemistry Education, Chungbuk Natioanl University, Korea
[1]*Division of Science Education, Daegu University, Korea*

Though the overseas voluntary activities are increasing in Korea recently, there is still the negative perceptions on going abroad for voluntary activities. Korean secondary school teachers and professors had gone to Timor-Leste and performed the voluntary activity of science education from 2007 to 2016. This study aims to help people's understanding on voluntary activity by finding meanings of this activity and sharing the lives of participants of this activity while looking through their stories of participation. We gathered the interview data for 8 participants in 2016, the note of participant observation of one author, the SNS documents, the photographs, the essays etc. and analyzed the data by the consecutive comparative analysis. We searched the meaning of this voluntary activity by answering such questions as 'why did you go to Timor-Leste?', 'what did you do there?', 'what was the reason of doing voluntary activity continuously?', 'what did you feel?', and 'what was changed in yourself?'. The driving forces of the continuation of this activity of doing science experiment with Timor-Leste teachers were 'keeping promise', 'trust on people' etc. The participants experienced various changes such as 'regaining smile', 'enforcing passion and self-confidence', 'rediscovering the importance of science education' etc. This activity showed all the characteristics of voluntary activity reported in the literature, and in addition, gave the implications on the necessity of voluntary activity focused on science education. This voluntary activity had kept all the participants' lives warm. [This work was supported by the Ministry of Education of the Republic of Korea and the National Research Foundation of Korea (NRF-2015S1A5A2A03048047)]

Poster Presentation : **EDU.P-536**

Chemistry Education

Zoom 10 WED 16:30~17:00

Activities to commemorate the 150th anniversary of Mendeleev's discovery of the periodic table of the chemical elements

Young Tae Kong

Science Education, Chinju National University of Education, Korea

In this presentation, in order to commemorate the 150th anniversary of Mendeleev's discovery of the periodic table of the chemical elements, I would like to introduce the ‘Life Chemistry’ class given to first-year undergraduates in 2018 and 2019. In this class, the class was conducted from the viewpoint of the discovery and history of chemical elements, and as the output of the course, students submitted their own chemical elements. In addition, they performed activities to express their English name only with chemical element symbols.College students who participated in this class tried to express their own ideas on one page of paper, briefly explaining the physical and chemical properties of each chemical element in charge, using pictures and letters. These activities helped pre-service teachers not only to understand the concept of chemical elements, but also to understand the world through elements.

Poster Presentation : **EDU.P-537**

Chemistry Education

Zoom 10 WED 16:30~17:00

A study on the contents of articles about chemical elements published in Hansung Sunbo newspaper

Young Tae Kong

Science Education, Chinju National University of Education, Korea

The purpose of this presentation is to obtain basic data on the changes of chemical elements in the late Joseon Dynasty in terms of acceptance of modern civilization. To achieve this purpose, the newspaper of Hanseong Sunbo which first awakened the concept of chemical elements to the public at the end of the 19th century, was analyzed. Among these articles, a review was conducted on the contents of the Korean translations for five articles (hydrogen, carbon, oxygen, nitrogen, and chlorine).Through this review, two serious errors were found in Hanseong Sunbo's Korean translation, and five cases were identified that were not translated. In addition, 20 other areas requiring correction were found.

Poster Presentation : **EDU.P-538**
Chemistry Education
Zoom 10 WED 16:30~17:00

the Effects of Collaborative Problem-solving for Character Competence (CoProC) instruction model on Character Competence of Elementary School Students

Jaekyoung Jun, Geonu Kim, Jihun Park, Eugene Kang[1], Jiaeng Park[2], Jeonghee Nam[2,*]

Department of Chemistry Education, Pusan National University, Korea
[1]*Pusan National University, Korea*
[2]*Department of Chemical Education, Pusan National University, Korea*

The purpose of this study was to investigate an impact of the Collaborative Problem-solving for Character Competence (CoProC) instruction model to elementary school science classes. The Collaborative Problem-solving for Character Competence (CoProC) instruction model was developed to foster character competence within the context of secondary science education. In order to apply the CoProC program for elementary school students, five CoProC activities were developed that can be implemented within the context of elementary science education and twenty-six fifth grade students were participated in this study. The Character Competence Test was administered before and after the intervention and students' reflective writings were collected and analyzed. In order to investigate the difference between school levels, it was compared with the results of previous research that applied to middle and high school students.

Poster Presentation : **EDU.P-539**
Chemistry Education
Zoom 10 WED 16:30~17:00

The Impact of Negotiation-Based Self and Peer Assessment Activities on Science-Gifted Students' Science Writing and Multiple Representation

Eunbi Jo, Dojun Jung, Jeonghee Nam[1,*]

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

The purpose of this study was to examine the impact of Negotiation-Based self and peer assessment activities on science-gifted students' science writing and multiple representations. The participants of this study were 93 11th grade students (five classes), and students were taught five subjects about 'enthalpy', 'equilibrium', 'acids and bases', etc. At the end of each class, students wrote science writing on each subject and then conducted self and peer assessment. Science writing was evaluated based on the criteria derived by students' negotiations, the result of self and peer assessment of science writing were analyzed to examine the changes in science writing. Then we used surveys and interviews to check the validity of self and peer assessment activities. Also, to study how the self and peer assessment activities influenced the multiple representations, we analyzed students' science writing using the multiple representations analyze framework developed by Nam *et al*.(2001). Based on the results, this study would like to suggest a learning environment that supports 'student agency' in learning outcomes as well as the learning process.

Poster Presentation : **EDU.P-540**
Chemistry Education
Zoom 10 WED 16:30~17:00

Errors and Mistakes in Students' Research Reports at National Science Exhibition

Ju Ran Shin, HyunJu Park[1,*]

Department of Chemical Education, Chosun University, Korea
[1]*Faculty of Science Education, Chosun University, Korea*

The purpose of this study was to investigate students' research results report and analyze errors in the process of students performing research or writing in the report. The results of this study would help us to understand the difficulties in the process of students conducting free inquiry research activities. In addition, it was expected that teachers could be used as basic data for teaching students' free inquiry research. A total of 60 students’ reports from 23 elementary schools, 13 middle schools, and 24 high schools out of 300 reports in 8 fields of Chemistry, Environments, Industry and Energy, Physics, Animals, Earth Science, Agriculture, Forestry and Fisheries, and Plants and that received the Encouragement Award at the 2018 National Science Exhibition. The following errors or mistakes were found in students' reports: Hypothesis setting; setting of experimental group and comparative group; setting variables such as dependent variable, independent variable, and control variable; consider limited conditions; understanding of prior research; number of experiments, and etc.

Poster Presentation : **EDU.P-541**

Chemistry Education

Zoom 10 WED 16:30~17:00

Excitation spectrum, nanoparticles, and their applications in cellular optical imaging

Sungjay Hong, Yanlu Zhao, Sungmoon Choi, Junhua Yu[*]

Department of Chemical Education, Seoul National University, Korea

The attractive photophysical properties of luminescent nanoparticles have prompted numerous studies on their synthesis and biological applications. Because of the complexity of components, sizes, morphologies, and strong light scattering of the nanoparticles the absorption spectrum alone is not enough for characterising and analysing the real absorption band of a nanoparticle product. Instead, the excitation spectrum is necessary for this purpose. To address the importance of the excitation spectrum in the utilisation of the photophysical properties of nanoparticles for cellular imaging, we compared the absorption and excitation spectra of a small organic molecule (rhodamine 6G) and commercially available nanoparticles (semiconductor quantum dots). Rhodamine 6G shows a good superimposition between its absorption and excitation spectra. However, the quantum dots do not, due to the presence of impurities and the polydispersity in nanoparticle size and shape. We demonstrated, by either spectrometer or cellular imaging, that excitation of the quantum dots at the maximum absorption peak will not result in the highest emission intensity. Instead, the best excitation wavelength for the nanoparticles can be revealed by the excitation spectrum. This has usually been overlooked by chemists and biologists.

Poster Presentation : **EDU.P-542**
Chemistry Education
Zoom 10 WED 16:30~17:00

Applying Chemistry Knowledge to Arduino-Neutralization Titration

Pil-Kwang Oh, Seong-Joo Kang*

Department of Chemical Education, Korea National University of Education, Korea

The Physical computing and Coding education are receiving a lot of attention in various fields. In the educational field, the need for education utilizing Physical computing and Coding education are also being emerged. In this study, we have created a new type of the Arduino−Neutralization Titration experiment device that is operated by manipulating the code. The traditional neutralization titration experiment uses indicator or pH meter to calculate the concentration of acid and base. The indicator do not have a constant discoloration because it cause accidental error and is not manufactured in the same environment. And the pH meter cannot operate the program inside the device, so only simple measurement is possible. However, the Arduino−Neutralization Titration is designed with LED and pH sensor, and the LED acts as an indicator as color changes depending on the pH value. In addition, this device has a discoloration range of three indicators, allowing you to select the indicator depending on your experiment. Above all, students can understand scientific concepts while interpreting code, and can easily manipulate code, enabling various thinking. Therefore, we would like to suggest that the Arduino−Neutralization Titration be used at schools to enhance students' understanding of scientific concepts and to help expand their thinking.

Poster Presentation : **ENVR.P-543**
Environmental Energy
Zoom 10 WED 17:00~17:30

Highly efficient perovskite solar cells with novel dopant-free polymeric hole transport material

Dohyun Kim, Junwoo Lee, Kyoungwon Choi, Hae Un Kim, Taiho Park*

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

Charge transport layer Is crucial for obtaining high efficiency in organic-inorganic hybrid perovskite solar cell. Especially, hole transport layer (HTL) plays more important role in n-i-p perovskite solar cell structure, because it should protect perovskite layer from external oxygen and moisture. Thus, it is necessary to develop dopant-free polymeric hole transport material (HTM) to get hydrophobicity and stability of HTL. Herein, we synthesized novel donor-acceptor type polymeric HTM (PTEG) By introducing tetraethylene glycol (TEG) side chain in BDT-BT based conducting homopolymer, we improved solubility of HTM and increased hole mobility due to increasing π- π stacking of polymer, confirmed with grazing-incidence wide-angle X-ray scattering (GIWAXS) and space charge limited currents (SCLC). As a result, we demonstrated n-i-p type perovskite solar cell using our polymer, achieving 19.8% power conversion efficiency without using dopant. Furthermore, compared to spiro-OMeTAD, ambient stability noticeably increased, almost no loss of efficiency after 200 hours at 25% relative humidity and room temperature.

Poster Presentation : **ENVR.P-544**

Environmental Energy

Zoom 10 WED 17:00~17:30

A study on the durability enhancement of PtCo/C in PEMFC cathode by including dissolved Co^{2+} capturing layer

Youjin Lee, Kahyun Ham[*], Jaeyoung Lee[1,*]

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Fuel cell produces electric energy from chemical energy, which comes from hydrogen and oxygen. There are many types of fuel cells depending on electrolyte. One of them is proton exchange membrane fuel cell (PEMFC). PEMFC operates in low temperature and its electronic density is high. Additionally, it does not produce carbon dioxide (CO_2) during operating, it is known as one of the environmentally friendly energy systems. During PEMFC operation, oxygen reduction reaction has higher overpotential because of its slow reaction rate. Therefore, Pt-based metal catalysts are commonly used for fastening ORR rate. Both ORR activity and price competitiveness are need to be enhanced, 4d transition metals (e.g. Co, Ni, Fe) are alloyed with Pt. While its better performance, transition metals are easier to be dissolved than Pt in PEMFC operating condition, they cause deactivation of PEMFC performance.In this study, we tried to get higher durability of the PtCo/C catalyst in PEMFC cathode by capturing dissolved Co^{2+} ion. N-doped carbon layer, made of mainly pyridinic N is added to capture dissolving Co^{2+} ion. We observed oxidation peak in cyclic voltammetry to confirm whether Co^{2+} is captured. Then, we compared ORR performance difference depending on the amount of N-doped carbon. Also, accelerated stress test was conducted to evaluate the durability of catalyst with N-doped carbon.

Poster Presentation : **ENVR.P-545**

Environmental Energy

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Effects of metal oxide nanoparticles for thermally stable planar perovskite solar cells

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Perovskite solar cells (PSCs) have been considered next-generation energy harvesting applications, however, the low stability of perovskites under a harsh environment impedes the commercialization of PSCs. We found that the temperature of the perovskite layer increases rapidly under light irradiation, and for this reason, the continuously accumulated heat adversely affects the device performance. To solve this problem, we employed metal oxides nanoparticles to control the thermal behavior of hole-transporting materials (HTMs). As a result, we demonstrated a PSC retaining 91% of its initial efficiency under a harsh condition (high temperature and high humidity) after 31 days. We tested our approach using several HTMs and confirmed that the same enhancement in thermal stability was achieved regardless of the HTMs. This means our strategy has a great potential for developing thermally stable PSCs.

Poster Presentation : **ENVR.P-546**

Environmental Energy

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Precursor Engineering by using the PbI_2-DMSO complex and Fabrication of Highly Efficient Perovskite Solar Cells.

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Perovskite solar cells have been researched intensively due to their superior optoelectronic properties such as long carrier diffusion length, ambipolar charge transport, and high absorption coefficient as well as solution-processability. In order to unlock the full potential of perovskite materials itself, the uniform formation of perovskite thin film should be preceded. High quality of the perovskite film can be achieved by precise control of a solution dispersion state because the final film morphology is directly transferred from the perovskite precursor colloids in the solution..In this work, the PbI_2-DMSO complex were synthesized and used as a precursor instead of direct dissolution of PbI_2 in DMSO. The chemical and physical properties of the PbI_2-DMSO complex were investigated by various characterization methods such as particle size analysis, UV-Vis, SEM, and FT-IR. The homogeneous dispersion of perovskite precursor in a solution by using PbI_2-DMSO complex enabled a formation of high-quality perovskite film with large grain-size. As a result, the device performance was improved by using PbI_2-DMSO complex, mainly originated from the enhanced open-circuit voltage.

Poster Presentation : **ENVR.P-547**
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Application of Methanol-tolerant Pt Catalyst with Phosphorus-doped Carbon Layer on Direct Methanol Fuel Cell

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Global warming, which has become severe in recent years, is threatening human life, and fuel cells are excellent alternative energy for fossil energy. Among various types of fuel cells, direct liquid fuel cell, especially direct methanol fuel cell (DMFC) is quite attractive technology due to various advantages of rapid refueling and high energy density, which are crucial characteristics for portable applications. DMFC consists of methanol oxidation reaction at anode and oxygen reduction reaction (ORR) at cathode on PtRu-based and Pt-based catalyst, respectively. One of the most challenging problems toward DMFC is methanol crossover. Methanol at the anode permeates the cathode and reacts with cathode catalyst, resulting in voltage drop. Pt/C is an excellent catalyst, but it actively reacts with methanol at the cathode. Thus, methanol-tolerant property has great significance with Pt-based catalyst to increase the ORR selectivity at the cathode. In our previous study, we synthesized Pt catalyst with N, P-doped carbon layer. We found out that Pt catalyst with phosphorus doped carbon layer has the potential for methanol tolerance, maintaining the ORR activity with addition of methanol. Therefore, we focus on Pt/C-P catalyst this time. Pt/C-P showed both lower activity in the methanol oxidation reaction and higher activity in ORR than pristine Pt/C. The excellent selectivity toward ORR of Pt/C-P would be originated from phosphorus-doped carbon layer, blocking the diffusion of methanol. Finally, we will apply heteroatom-doped Pt/C on the cathode and confirm selectivity compared with pristine Pt/C. This approach suggests the way to design a Pt catalyst for ORR to improve performance in DMFC.

Poster Presentation : **ENVR.P-548**
Environmental Energy
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Moderate Oxophilic CoFe in Carbon Nanofiber for the Oxygen Evolution Reaction in Anion Exchange Membrane Water Electrolysis

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We propose corrosion-resistant carbon-coated Co0.9Fe0.1 alloy nanoparticles as highly active and durable electrocatalysts for the oxygen evolution reaction (OER) in anion exchange membrane water electrolysis (AEMWE). In the presence of 10% Fe atoms, the oxophilicity of Co metal is modulated in a direction to facilitate OH- adsorption on Co3+; thus, Co0.9Fe0.1-carbon nanofiber (CNF) can exhibit smaller overpotentials than other metal ratios in Co1-xFex-CNF. Additionally, we confirm catalytic degradation from the oxidation of the carbon layer, which is triggered by defects in the carbon originating from Fe during the pyrolysis step. The Co0.9Fe0.1 metal is further optimized by increasing graphitization to simultaneously achieve superior activity and durability for application on AEMWE. This work not only demonstrates the role of Fe in Co metal for controlling the proper oxophilicity but also shows the importance of graphitized carbon as a catalyst support for stable water oxidation.

Poster Presentation : **ENVR.P-549**
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Cobalt-Antimony Oxide for Oxygen Evolution Reaction in Anion Exchange Membrane Water Splitting

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Electrochemical water splitting is the one of the promising ways to obtain hydrogen from aqueous media. Oxygen evolution reaction (OER) at the anode is the rate-determining step due to the sluggish kinetics, which leads to reducing energy efficiency. Recently, anion exchange membrane water splitting has been considered as an alternative way because of its capability of producing hydrogen of high purity and the availability of iron-triad element-based catalysts because of their thermodynamically stability in alkaline media. Besides, cobalt oxides such as spinel, layered double hydroxide are being investigated as active OER electrocatalyst. Among them, the spinel-type Co_3O_4, which contains one Co^{2+} in the tetrahedral site and two Co^{3+} ions in the octahedral site, exhibits outstanding OER performance in alkaline media and has been actively investigated.In this study, we investigated cobalt-antimony oxide as OER catalyst in alkaline media, which has unique crystal structure and contains abundant octahedral Co^{2+} compared to spinel-type cobalt oxide. We aimed at identifying the role of octahedral Co^{2+} of cobalt-antimony oxide by using in-situ X-ray absorption near-edge structure analysis. We also carried out anion exchange membrane water splitting to confirm the availability as the anode catalyst to produce H_2 gas.

Poster Presentation : **ENVR.P-550**

Environmental Energy

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Development of a colorimetric detection method of chlorine dioxide ions using recyclable concave cubic gold nanoparticles

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The present study reported on the qualitative and quantitative detection of chlorine dioxide ions, which are harmful substances contained or dissolved in oxidizing agents. We developed a colorimetric detection method of chlorine dioxide ions using concave cubic gold nanoparticles, and in more detail, biological samples, drinking water, environmental samples and antibiotics. Chlorine dioxide ions etched AuNCs which changes the deep blue color to pink. The prepared particle was characterized by UV–visible spectrophotometer, Transmission electron microscope (TEM), particle size analyzer and zeta sizer. The diameter of synthesized nanoparticle particle was measured by using particle size analyzer and it was found to be 40 ± 1.3 nm. The surface of the cubic-shaped nanoparticles is transformed into spherical nanoparticles as chlorine dioxide ions are continuously etched. Surface Plasmon Resonance, such as concave cubic gold nanoparticles, appears and emits a specific wavelength through the etching process by chlorine dioxide ions and changes in size and shape of the particles. This present study can be applied in various ways to sensors that measure and monitor environmental pollutants.

Poster Presentation : **ENVR.P-551**
Environmental Energy
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Highly sensitive gas sensor using graphene doped with ZnO nanosheet for detection of NO2 gas

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The current research is focusing on the charateristic of ZnO nanosheets on graphene using spin coating technique for the fabrication of NO2 gas sensors. Physical properties for graphene composite doped with ZnO nanosheet have been intensively investigated using electron microscopy and various spectroscopies. Doping with ZnO nano sheets induced to change electronic properties of graphene, and it led to alter drastically resistivity of graphene in the presence of NO2 gas. Graphene doped with ZnO nano sheets demonstrated the ability to sense NO2 gas sensitively with the saturation time is around 400s, and with the limit of detection being below 0.15ppm. In comparison with other gases this sensor has very good selectivity and repeatedly.

Poster Presentation : **ENVR.P-552**

Environmental Energy

Zoom 10 WED 17:00~17:30

Oxygen vacancy control on cerium oxide for mild photocatalytic oxidation

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A simple pH treatment in synthetic environment successfully tuned the oxygen vacancies in cerium oxide. The amount of oxygen vacancies in CeO_2 is altered via a facile strategy by modifying pH condition of synthesizing media (i.e. acid (CeO_2-A) and base treatment (CeO_2-B)) without adding further co-catalysts or chemicals. The superior photocatalytic degradation (PCD) rates of CeO_2-B comparing to CeO_2-A (~1.5 times) indicated that exceptionally stable oxygen vacancies were successfully generated using the base treatment condition. Engineered oxygen vacancy is able to couple with solar energy to generate reactive oxygen species (ROS) during the photocataytic wastewater treatment. The selective PCD activities of CeO_2-A and CeO_2-B in the degradation of a variety of aromatic substrates in water were determined, affirming that the operating mechanisms for UV-illuminated CeO_2 are very different from those of TiO_2 photocatalyst.

Poster Presentation : **ENVR.P-553**
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Modeling of mercury mass and isotopic transport by species in lake

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To date, various lake mercury cycle models have been developed to understand the various factors that influence mercury concentrations in lakes. However, no model has been made to simulate the behavior of mercury stable isotopes in lakes. In this study, we develop a model that can simulate not only the mass of mercury but also the isotopic transport in lakes. Atmospheric mercury deposition which represent one of the main mercury inputs to lake environments are obtained by simulating the Global Atmospheric Chemical Transport Model (GEOS-Chem). Different atmospheric mercury deposition results can be applied to our lake model to represent various lakes and simulate mercury cycle under different mercury reduction scenarios. Our lake model comprises three mercury species which include Hg^0, Hg^{2+}, and Hg_P, and the layers are divided into epilimnion, hypolimnion, surface sediment, and deep sediment to create a model consisting of a total of 12 ordinary differential equations. Rate coefficients representing each transport process (k, yr^{-1}) are gathered from the literature. The model will be calibrated based on the results of concentration and isotopic studies in the Lost Lake in Wyoming, USA. Various scenarios will be simulated for different lake environments in various regions. Changes in mercury concentrations in lake sediments can be projected to compare reaction times for mercury reduction in sediments under different scenarios, and isotope analysis will be used to predict which transport processes have the greatest impact on mercury deposition. Ultimately, this can suggest appropriate mercury reduction regulations and expected outcomes specific for each region.