133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Plenary Lecture : **PLEN-1**

Plenary Lecture

Convention Hall 2 THU 13:30

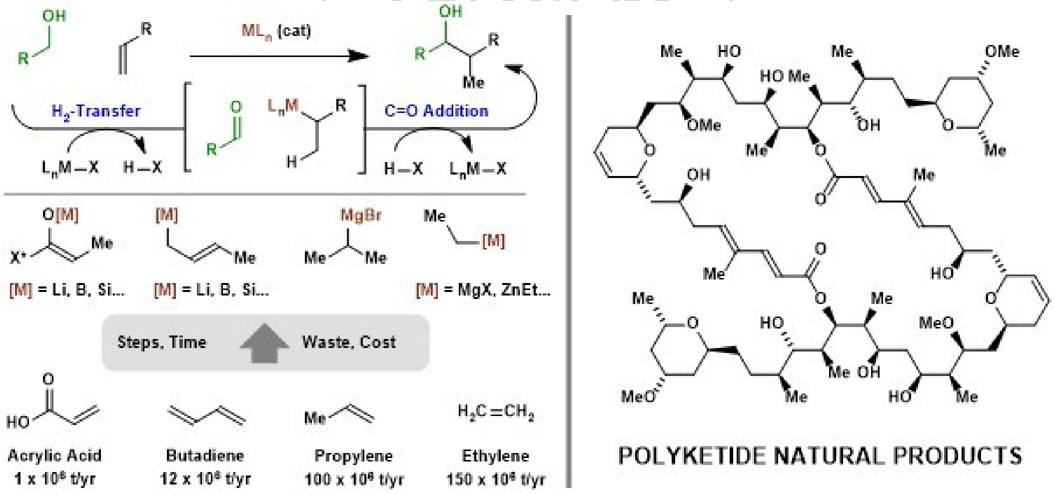
Chair: Soo Bong Han (KRICT)

Catalytic C-C Coupling of Alcohols via Hydrogen Auto-Transfer: Reinventing Carbonyl Addition

Michael J. Krische

Department of Chemistry, The University of Texas at Austin, United States

Research in the Krische group is focused on the development of catalytic methods for C-C bond formation that occur through the addition or redistribution of hydrogen. This work includes the first H2-mediated carbonyl reductive couplings beyond hydroformylation, and related hydrogen auto-transfer reactions where alcohols function as both reducing agents and carbonyl proelectrophiles. Carbonyl addition via hydrogen auto-transfer enables byproduct-free conversion of lower alcohols to higher alcohols. The development of these methods, the influence of metal-centered stereogenicity on regio- and enantioselectivity, and the application of these methods to polyketide total synthesis will be described.



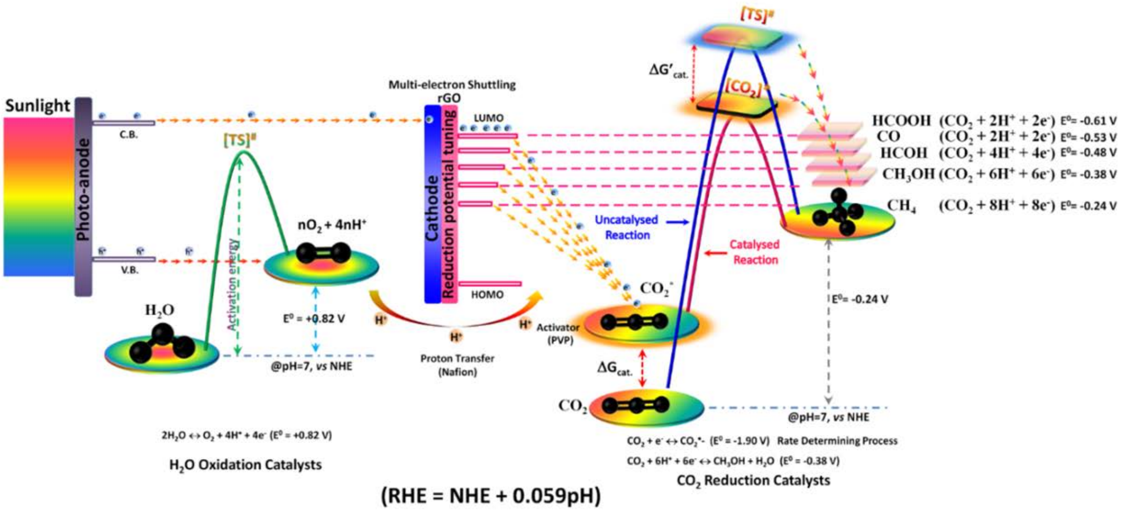
Award Lecture : **AWARD1-1**
Award Lecture - 2024 Academic Excellence Award
Room 304+305+306 FRI 13:30
Chair: Seunghoon Shin (Hanyang University)

Carbon Neutrality Climate Technology Based on Nanotechnology

Young soo Kang

Environmental & Climate Technology, Korea Institute of Energy Technology (KENTECH), Korea

In this talk, approaching technology on the photoelectrochemical and photochemical CO2 reduction reaction to have higher solar to fuel efficiency than 2.0% will be introduced. To have such as high efficiency, several parameters for the thermodynamics and kinetics control were optimized in both approaches such as multi-electron shuttling process, reduction potential tuning, CO2 activation and multiple proton-coupled multiple electron transfer process as one pot reaction. Basically, CO2 reduction can be done combined with two water splitting reaction to produce maximum of electrons and protons to supply for CO2 reduction reaction. To have maximum of electrons and protons, we have tried with more than 30 kinds of photocatalysts and decided that BiVO4 was the best one as the pristine photocatalyst. By using BiVO4, we also added some more functional approaches to increase the efficiency of water splitting reaction via band gap engineering, crystal facet engineering and interface junction engineering. All of these technologies could be achieved based on the physical chemistry by optimizing parameters of the materials an process. Further more work is going on continuous flow process for mass production.


Sunlight
Photo-anode
C.B.
V.B.
$[TS]^{\#}$
Activation energy
H_2O
$nO_2 + 4nH^+$
$E^0 = +0.82$ V
@pH=7, *vs* NHE
$2H_2O \leftrightarrow O_2 + 4H^+ + 4e^-$ ($E^0 = +0.82$ V)
H_2O Oxidation Catalysts
Multi-electron Shuttling
rGO
Cathode
Reduction potential tuning
LUMO
HOMO
H^+
H^+
H^+
Proton Transfer
(Nafion)
Activator
(PVP)
(RHE = NHE + 0.059pH)
$[TS]^{\#}$
$\Delta G'_{cat.}$
$[CO_2]^{*}$
$CO_2^{\cdot}$
$\Delta G_{cat.}$
CO_2
Uncatalysed
Reaction
Catalysed
Reaction
HCOOH ($CO_2 + 2H^+ + 2e^-$) E^0= -0.61 V
CO ($CO_2 + 2H^+ + 2e^-$) E^0= -0.53 V
HCOH ($CO_2 + 4H^+ + 4e^-$) E^0= -0.48 V
CH_3OH ($CO_2 + 6H^+ + 6e^-$) E^0= -0.38 V
CH_4 ($CO_2 + 8H^+ + 8e^-$) E^0= -0.24 V
E^0= -0.24 V
@pH=7, *vs* NHE
$CO_2 + e^- \leftrightarrow CO_2^{\cdot -}$ ($E^0 = -1.90$ V) Rate Determining Process
$CO_2 + 6H^+ + 6e^- \leftrightarrow CH_3OH + H_2O$ ($E^0 = -0.38$ V)
CO_2 Reduction Catalysts

Award Lecture : **AWARD2-1**

Award Lecture - 2024 Man Jung Han Academic Excellence Award

Room 304+305+306 WED 13:00

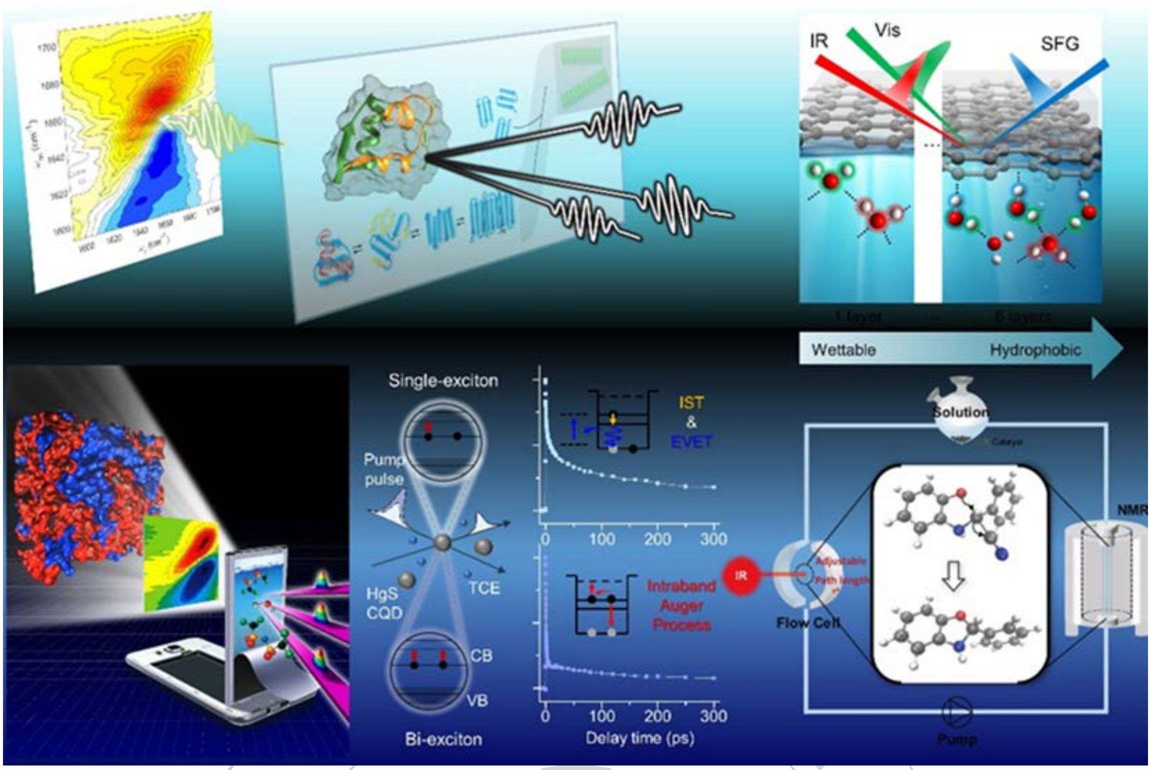
Chair: Changsik Song (Sungkyunkwan University)

In-Operando Time-resolved Vibrational Spectroscopy

Kyungwon Kwak

Department of Chemistry, Korea University, Korea

The time-resolved ultrafast nonlinear infrared (IR) spectroscopy has been contributed to studies of molecular dynamics and various chemical reactions such as energy transfer, proton hopping, protein denaturation, and chemical exchanges. With the advances in laser technology and optics, there has been improvements in spectral- and time-resolution, signal to noise ratio, and spatial resolution through adapting the development in microscopies. However, the application of advanced spectroscopies and microscopies still have been limited to studies of samples optimized for spectroscopic observation rather than function or performance of the sample. To expand the application of time-resolved vibrational spectroscopies, we have been developing various methods to combine chemical reactor, a living cell, and electronic devices with nonlinear spectroscopies like polarization selective pump-probe (IR-PP), transient two-dimensional IR (2D-IR), IR-Vis sum-frequency generation (SFG), two-dimensional electronic spectroscopy (2D-ES). In this talk, a couple of application will be discussed; 1) solvation structure and dynamics of electrolytes in Li-ion battery 2) wettability of graphene and interfacial water structure observed with vibrational SFG 3) phase separation in highly concentrated aqueous electrolytes for a lithium-ion battery 4) Protein aggregation dynamics with 2D-IR.


IR
Vis
SFG
1 layer
6 layers
Wettable
Hydrophobic
Single-exciton
Pump pulse
HgS CQD
TCE
CB
VB
Bi-exciton
IST & EVET
Intraband Auger Process
0
100
200
300
Delay time (ps)
Solution
Catalyst
NMR
IR
Adjustable Path length
Flow Cell
Pump

Symposium : **KCS1-1**
[BKCS Symposium] BKCS: The Cornerstone of Korean Basic Science
Room 301+302 WED 14:00

New Era for BKCS

Myung Hwan Park

Department of Chemical Education, Chungbuk National University, Korea

The Bulletin of the Korean Chemical Society (BKCS) is the flagship journal of the Korean Chemical Society (KCS), founded in 1980 to share new findings in all chemical sciences. All BKCS papers published on Wiley Online Library with the support of the KCS are strictly peer-reviewed. The BKCS journal welcomes Communications, Articles, Personal Accounts, and Reviews written in English. The BKCS covers all fields of chemistry, including analytical chemistry, electrochemistry, industrial chemistry, inorganic chemistry, life-science chemistry, macromolecular chemistry, organic synthesis, non-synthetic organic chemistry, physical chemistry, and materials chemistry. In this talk, BKCS's current state, the history, and future strategy heading into a new era will be presented.

Symposium : **KCS1-2**

[BKCS Symposium] BKCS: The Cornerstone of Korean Basic Science

Room 301+302 WED 14:30

Chair: Eunsung Lee (Seoul National University)

Exploring Strategies for Noncentrosymmetric Solid-State Materials: From Chromophore Incorporation to Systematic Design

Kang Min Ok

Department of Chemistry, Sogang University, Korea

The attention directed towards functional inorganic materials forming noncentrosymmetric (NCS) crystalline structures is fueled by their diverse structure-related properties, encompassing pyroelectricity, piezoelectricity, second-harmonic generation, ferroelectricity, and multiferroic behavior. These materials hold substantial promise for practical applications in medical lasers, telecommunications, lithography, detectors, energy harvesting, and data storage. However, the challenge persists in enhancing the feasibility of creating macroscopic NCS structures within synthetic solid-state materials.One successful strategy involves incorporating NCS chromophores, such as polyhedra featuring cations prone to second-order Jahn-Teller distortions, highly polarizable metal cations, and π-conjugated asymmetric anions with trigonal planar geometry. Unfortunately, the prevalent tendency of reaction products is to adopt centrosymmetric structures, possibly influenced by nature's inclination towards symmetry.In this presentation, we delve into key factors influencing framework structures and macroscopic centricity through meticulous structural analyses of recently reported materials containing asymmetric building units. Additionally, we propose systematic approaches aimed at the discovery of functional solid-state materials with noncentrosymmetric structures.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

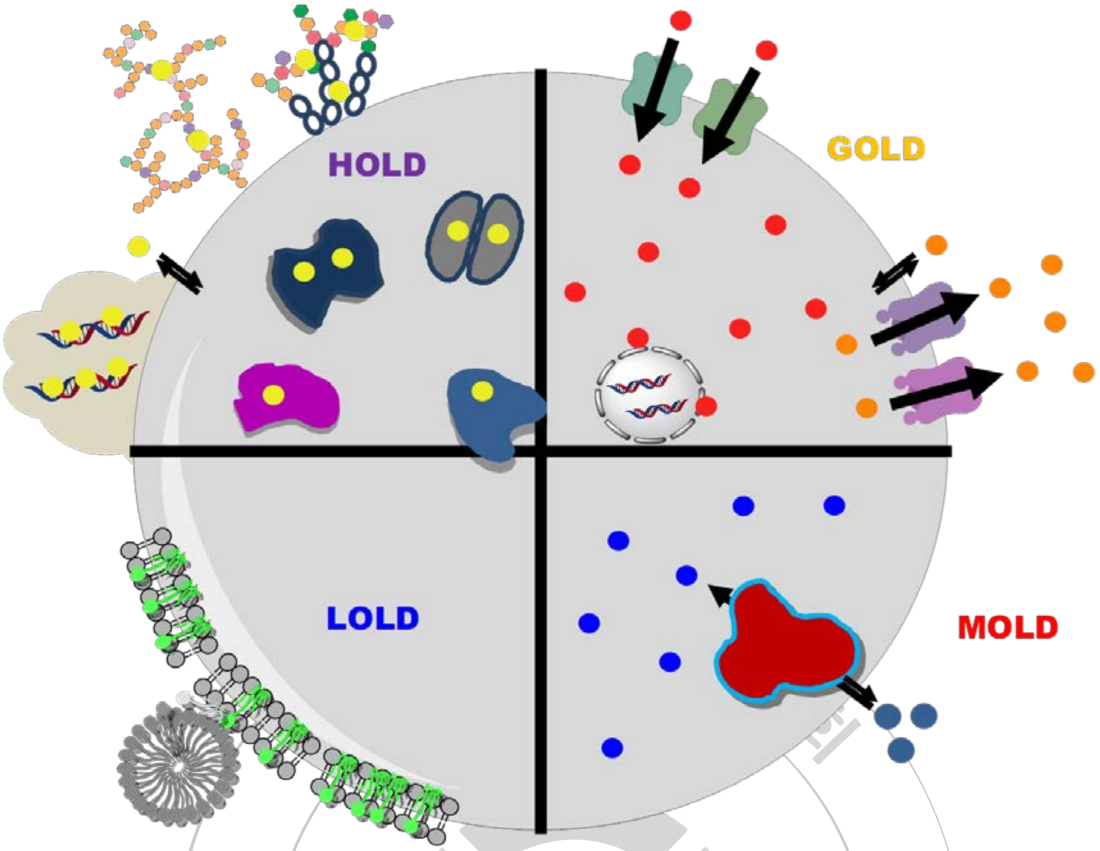
Symposium : **KCS1-3**
[BKCS Symposium] BKCS: The Cornerstone of Korean Basic Science
Room 301+302 WED 14:55
Chair: Eunsung Lee (Seoul National University)

Live cell distinction using organic fluorescent probes

Young-Tae Chang

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

Accurately discerning between diverse cell types within multicellular organisms is fundamental for unraveling intricate cellular interactions and regulatory mechanisms. Conventional methods predominantly rely on antibodies targeting specific biomarkers on cell surfaces. However, to surmount limitations associated with antibody-based approaches, we have developed a series of small fluorescent probes capable of live-cell distinction. These probes encompass Protein Oriented Live-cell Distinction (POLD), Carbohydrate Oriented Live-cell Distinction (COLD), Gating Oriented Live-cell Distinction (GOLD), and Lipid Oriented Live-cell Distinction (LOLD), targeting proteins, carbohydrates, membrane transporters, and lipid compositions, respectively. Our recent advancement, Metabolism Oriented Live-cell Distinction (MOLD), extends the repertoire by focusing on metabolic signatures of cells. Through elucidating the design and mechanisms underlying these probes, particularly in immune cell populations, novel insights have emerged, paving the way for the development of more selective and comprehensive cell distinction tools. The multidimensional layer of our approach promises to provide invaluable insights into characterizing complex cell communities.


HOLD
GOLD
LOLD
MOLD

Symposium : **KCS1-4**

[BKCS Symposium] BKCS: The Cornerstone of Korean Basic Science

Room 301+302 WED 15:20

Chair: Eunsung Lee (Seoul National University)

Biosynthetically Inspired Synthesis of Complex Natural Products

Sunkyu Han

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

The field of total synthesis of natural products has witnessed remarkable progress throughout the past century. Thanks to the collaborative efforts of the synthetic community, intricate targets have been successfully synthesized through innovative solutions. These solutions, in turn, have laid the foundation for developing new drugs and materials. As expectations for synthetic organic chemists continue to rise, the role of total synthesis is multifaceted: it serves as a driving force for discovering novel synthetic strategies, provides a platform for uncovering unprecedented bond formations through novel reactivities, enhances our understanding of biosynthetic machinery, and acts as a means to produce chemicals with extraordinary functions in substantial quantities. This dynamic evolution underscores the vital and expanding role that total synthesis plays in the realm of basic scientific discovery and application. In this presentation, I will delve into our group's latest findings in the field of total synthesis. The discussion will highlight how incorporating biosynthetic considerations can significantly accelerate the design and execution of complex secondary metabolite syntheses.

Symposium : **KCS1-5**

[BKCS Symposium] BKCS: The Cornerstone of Korean Basic Science

Room 301+302 WED 15:45

Chair: Myung Hwan Park (Chungbuk National University)

Electrosynthesis Promoting Sustainable Chemical Synthesis

Sang Hoon Joo

Department of Chemistry, Seoul National University, Korea

In the intersection of synthetic chemistry and electrochemistry, electrochemical synthesis emerges as a transformative field, leveraging the role of electrons to drive chemical transformations. Departing from conventional perspectives that conceive electrons as mere carriers of charge, this methodology orchestrates redox reactions to access value-added compounds from chemical feedstocks under mild, safe, and environmentally benign conditions. In the current era of severe climate change, the necessity to develop greener and more sustainable processes has become paramount. In this context, the discipline of electrosynthesis has attracted rejuvenated attention, ushering in a renaissance. This talk will introduce the current status of the field and present our group's works on the electrocatalytic synthesis of important commodity chemicals, including hydrogen peroxide, chlorine, and propylene oxide.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **KCS1-6**

[BKCS Symposium] BKCS: The Cornerstone of Korean Basic Science

Room 301+302 WED 16:10

Chair: Myung Hwan Park (Chungbuk National University)

Strategic Approaches to Developing MOFs with Novel Characteristics

Hoi Ri Moon

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

To develop metal-organic frameworks (MOFs) having novel properties, over the past two decades, many scientists in various fields have made intensive efforts. Recently, MOF-on-MOF architecture has been actively studied by combining two or more MOFs into a composite. Composite MOFs comprise one MOF and another material with noticeably different properties. Many researchers have integrated MOFs with other materials to produce new structures with synergetic properties. Unfortunately, in many of these composite MOFs, the precise nature of the interaction and the bonding at the interface between the two materials is unknown and cannot be characterized well by any of the known methods. In this talk, we present a joint computational/experimental workflow that screens thousands of MOFs and identifies the optimal MOF pairs that can seamlessly “connect” to one another by taking advantage of the fact that the metal nodes of one MOF can form coordination bonds with the linkers of the second MOF. Based on this synthetic strategy, we report the composites of dimensionally (2D and 3D) and functionally (conductive and porous) different two MOFs in the form of a well-integrated core-shell structure. The hierarchically assembled 2D-MOF@3D-MOF exhibits new interfacial properties that are responsible for synergetically enhanced sensing performances toward toxic H2S gas with the lowest recorded limit of detection, superior sensitivity, and outstanding selectivity at room temperature in air. Finally, we will introduce carboxylate-based MOF glasses, as a new class of materials, which show superior mechanical properties in hardness (H) and elastic modulus (E). Our research is the first step of carboxylate-based MOFs and sheds light on the viability of various meltable carboxylate-based MOFs.

Symposium : **KCS3-1**
[KCS-ACS Publications Summit] The Future of Transformative Molecules
Room 304+305+306 WED 14:00
Chair: Ein Jin Cho (Chung Ang University)

Design, Synthesis, and Implementation of Novel Tools to Probe Biological Questions

Erick M. Carreira

Department of Chemistry and Applied Biosciences, ETH-Zürich, Switzerland

The lecture will include discussion and analysis of recent natural product targets that have been synthesized in the group. It will focus on target-oriented synthesis as a driver for the generation of novel bioactive agents, methods and approaches. The methods involve novel and unexpected reactivity as well as unusual building blocks that are fully integrated to produce efficient synthetic pathways

Symposium : **KCS3-2**

[KCS-ACS Publications Summit] The Future of Transformative Molecules

Room 304+305+306 WED 14:40

Chair: Ein Jin Cho (Chung Ang University)

Metal-Oxygen Intermediates in Dioxygen Activation and Formation Reactions

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.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **KCS3-3**

[KCS-ACS Publications Summit] The Future of Transformative Molecules

Room 304+305+306 WED 15:40

Chair: Hye Jin Lee (Editor-in-Chief, JKCS /Kyungpook National University)

Direct Air Capture (DAC) of CO_2 with Porous Sorbent Materials Coupled with Scalable Processes

Christopher W. Jones

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, United States

Most current climate models suggest that limiting warming to $_2$ from the air, or “direct air capture” (DAC). Because of the ultra-dilute nature of air, the separation of CO_2 from this mixture presents a significant engineering challenge.

In this lecture, I will reflect on examples of STEM research successes targeting societal grand challenges, followed by a deep dive into the challenges of DAC. I will describe the design and synthesis, characterization and application of porous oxide-supported amine materials that we have developed as cornerstones of new technologies for the removal of CO_2 from air. DAC technologies offer an interesting case study for the parallel design of molecules, materials, unit operations, and processes in chemistry and chemical engineering.

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Symposium : **KCS3-4**
[KCS-ACS Publications Summit] The Future of Transformative Molecules
Room 304+305+306 WED 16:20
Chair: Hye Jin Lee (Editor-in-Chief, JKCS /Kyungpook National University)

Chemical Plasmonics with Metal Nanoparticles

Jwa-Min Nam

Seoul National University, Korea

Plasmonics deals with understanding and manipulating the interaction between light and matter at a scale that is significantly smaller than the wavelength of light (e.g., metal nanoparticles), and chemical nanoplasmonics is mainly about the study and use of nanoscale chemistry for advancing plasmonics and the use of plasmonics to address key issues and challenges in chemistry and other related fields. Designing, synthesizing and controlling metal nanostructures with a superhigh precision for a large number of structures are the keys to the reliable and widespread use of plasmonic nanostructures in chemistry, materials science, optics, nanoscience, biotechnology and medicine. Here, I will share the design, synthetic strategies and characterization results of molecularly tunable and structurally reproducible plasmonic nanostructures including metal nanogap structures, multi-component metal nanoparticles and gold nanocatenanes with strong, controllable and quantifiable plasmonic signals (e.g., quantitative surface-enhanced Raman scattering). I will then show their potential in addressing some of important challenges in plasmonics, biosensing, bioimaging and therapeutics, and discuss how these new plasmonic materials and platforms can lead us to new breakthroughs in nanochemistry, next-generation disease diagnostics, molecular computing and nanomachines/nanorobotics.

Symposium : **POLY1-1**
Recent Advances in Polymer Networks
Room 303 THU 15:40
Chair: Youn Soo Kim (POSTECH)

Structure and Chain Dynamics of Coacervate Core Hydrogel

Soo-Hyung Choi

Department of Chemical Engineering, Hongik University, Korea

Coacervation is a liquid-liquid phase separation when intermolecular interaction, such as charge-charge, cation-π, π-π, and hydrogen bonding, between macromolecules is active in aqueous media. Coacervates have a dynamically active liquid-like interior, stimuli-responsiveness, and low interfacial tension, which are helpful for various applications such as coatings, wet adhesives, and food processing. Coacervation phenomena can be judiciously incorporated into inhomogeneous polymers for controlled microphase-separated domains; representatives include micelles and hydrogels. The hydrophilic and charged nature of the coacervate cores enhances the transportation efficiency, cellular uptake, and stability of the loading compounds in various physiological conditions. However, much less is known about the dynamics of molecular partitioning in self-assembled structures, particularly molecular exchange aspects, yet this is the fundamental process to understanding stimuli-responsiveness, structural stability, and release of loading materials. This presentation addresses the chain dynamics of block copolymers in electrostatically associating hydrogels using model block polyelectrolyte systems. For spherical coacervate cores, chain movement perpendicular to the interface is crucial to achieve reproducible and equilibrium structures. We quantified the equilibrium dynamics by rotational rheology for hydrogel systems. The results provide key parameters to regulate the exchange dynamics and further insights to harness macroscopic changes of structural and mechanical properties in the electrostatically associating systems.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **POLY1-2**

Recent Advances in Polymer Networks

Room 303 THU 16:05

Chair: Youn Soo Kim (POSTECH)

Interfacial Complexation of Fixed Polymeric Ions in Polyelectrolyte Network Heterojunctions

HyeongJun Kim

Chemical and biomolecular Engineering, Sogang University, Korea

Ionoelastomers are liquid-free, soft, and single-ion conducting materials, in which one ionic species is anchored by the elastic network, while the other ion species is mobile. The heterojunction of ionoelastomers with opposite polarity yields an ionic double layer (IDL) at the interface, enabling the diode-like ionic current rectification. In this study, we demonstrate that ionic rectification of ionoelastomer heterojunction primarily originate from the solidification of polymeric ion complexes formed at the interface. When the reverse bias is applied, mobile counterions are pulled away from the interface and a reduced concentration of free counterions leads to the increase of glass transition temperature (Tg) of polymeric ion complexes in the IDL. As Tg approaches to room temperature, the interface undergoes glass solidification which inhibits the flow of the ionic current under reverse bias. When under forward bias, the drift of counterions toward the junction interfaces softens the complex, allowing the ionic current to pass through. The correlation between ion concentration and solidification of polymeric ions complexes is further investigated by the complex coacervation of corresponding polyanion and polycation polymerized ionic liquids (PILs). Our study suggests that soft ionic diode from the ionoelastomer heterojunction is primarily a kinetic process, arising from the solidification of the interfacial complex of polymeric ions.

133rd General Meeting of the Korean Chemical Society
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Symposium : **POLY1-3**
Recent Advances in Polymer Networks
Room 303 THU 16:30
Chair: Soo-Hyung Choi (Hongik University)

Bio-inspired Design of Hydrogel Robotics and the Use of Hydrogels for Studying Biology

Jae-Byum Chang

Korea Advanced Institute of Science and Technology, Korea

Hydrogels are promising materials for diverse applications, including biological applications such as carriers for drug delivery, scaffolds for tissue engineering, tissue adhesives, and even soft robotics. In this talk, I introduce two of our recent studies related to hydrogels. The first topic is the bio-inspired design of hydrogel grippers. The human hand is made of diverse materials with a wide range of material properties and functions, including bones, which have high strength and toughness and provide mechanical support to the body; muscles, which can rapidly contract in response to stimuli and enable the mechanical motions of the body; and cartilage, which is soft and connects bones to maintain the overall shape of the hand during motion. All three of these materials—bones, muscles, and cartilage—have high water content, yet the assembled hand exhibits a high level of load capacity. Here, we introduce our recent work on all-hydrogel grippers made by mimicking the structures of human hands. We used three hydrogels, each of which performs the role of bone, muscle, or cartilage. By employing a hydrogel adhesion strategy that strongly adheres these three hydrogels, we demonstrate an all-hydrogel gripper with a very high level of load capacity, capable of bearing more than 47.6 times its own weight. The second topic is the use of hydrogels for bioimaging. Biological systems, including cells and tissues, are composed of more than ten thousand different biomolecules, each with a size ranging from a few to tens of nanometers. The three-dimensional distributions and organization of these molecules are strictly controlled. To study biological phenomena, a technology that enables the visualization of such a large number of molecules at a single-molecule resolution is required. However, the resolution of optical microscopy is limited by the diffraction of light, which is not sufficient for this purpose. Here, we introduce our recent work on bioimaging using hydrogels. By forming swellable hydrogels inside target specimens and expanding the hydrogel-specimen composite, it is possible to expand specimens by more than 20-fold, enabling 20-fold higher resolution imaging of biological specimens using optical microscopy.

Symposium : **POLY1-4**

Recent Advances in Polymer Networks

Room 303 THU 16:55

Chair: Soo-Hyung Choi (Hongik University)

Activity-induced hopping diffusion of self-propelled particles in polymer networks

Jae-Hyung Jeon

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

The diffusion of tracer particles within polymer networks holds significant implications for a range of biological and industrial applications, from intracellular macromolecule transport to nanoparticle diffusion. While extensive research has been conducted in this area, the study of self-propelled particles navigating polymer networks has only recently emerged as a focal point within the field. In this talk, we present a series of computational studies focused on understanding the behavior of active tracers moving through polymer networks. Our investigations reveal that active tracers exhibit distinct diffusion behavior, characterized by activity-induced hopping diffusion, which differs markedly from diffusion driven solely by thermal energy. We quantitatively explore how physical parameters such as the mesh-to-particle size ratio, bending stiffness of the meshwork, and the Peclet number influence the dynamics of active tracers within the polymer network. Furthermore, we introduce an analytical theory to elucidate the phenomenon of active tracers escaping confinement within the meshwork, providing insights into the observed trapped times of active tracers. Additionally, we touch upon recent advancements in the field, including studies where the cross-linking of polymer networks can be disrupted by strong self-propulsion motion or where the polymer network is formed by random cross-linking.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

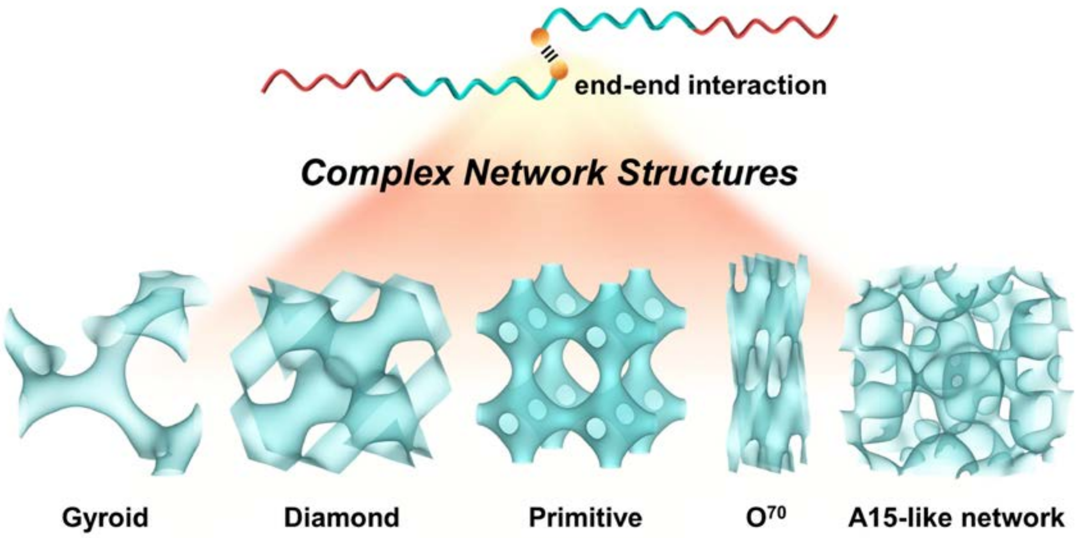
Symposium : **POLY2-1**
Special Symposium by Mid-Career Polymer Chemists
Room 303 FRI 09:00
Chair: Kyoung Taek Kim (Seoul National University)

End-group and Linker Chemistry in Polymer Science

Moon Jeong Park

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

The exploration of three-dimensional (3D) nanostructures in block copolymers involves the manipulation of compositional fluctuations at interfaces, induction of conformational asymmetry, and design of complex architectures. Despite the abundance of such nanostructures identified to date (e.g., triply periodic minimal surfaces and Frank–Kasper phases), the experimental demonstration of thermodynamically stable complex 3D structures with high packing frustration remains limited. In this talk, I would like to show the importance of molecular interactions for stabilizing complex 3D structures and proposes the use of end-group chemistry as a versatile method for realizing thermodynamically stable network structures with high packing frustration in simple linear diblock copolymers. I advocate revising conventional block-copolymer phase diagrams to consider end–end interactions and end-group arrangements. In instances where end-functionalized block copolymers exhibit strong end–end interactions, the lam structures are confined to a narrower phase diagram window. Conversely, a broader phase window enables the stabilization of diverse network structures such as gyroid, diamond, and primitive phases. This approach can reveal unprecedented network structures in various soft materials.


end-end interaction
Complex Network Structures
Gyroid
Diamond
Primitive
O70
A15-like network

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Symposium : **POLY2-2**
Special Symposium by Mid-Career Polymer Chemists
Room 303 FRI 09:25
Chair: Kyoung Taek Kim (Seoul National University)

Ionic conjugated polymers as a multifunctional interlayer for perovskite optoelectronic devices

Han Young Woo

Department of Chemistry, Korea University, Korea

To optimize the performance and stability of perovskite light-emitting diodes (PeLEDs) and solar cells (PeSCs), the incorporation of suitable charge transport layers (CTLs) and/or interlayers is essential. These CTLs must possess appropriate energy levels to facilitate efficient charge injection and transport, while effectively blocking opposite charges. Additionally, the CTL situated beneath the perovskite layer plays a pivotal role, significantly influencing the crystal growth of the perovskite layer and the presence of interfacial defects. In this presentation, a new series of ionic conjugated polymers will be discussed, commonly referred to as conjugated polyelectrolytes (CPEs) as ideal interfacial layers and CTLs for various PeLEDs and PeSCs devices.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **POLY2-3**

Special Symposium by Mid-Career Polymer Chemists

Room 303 FRI 09:50

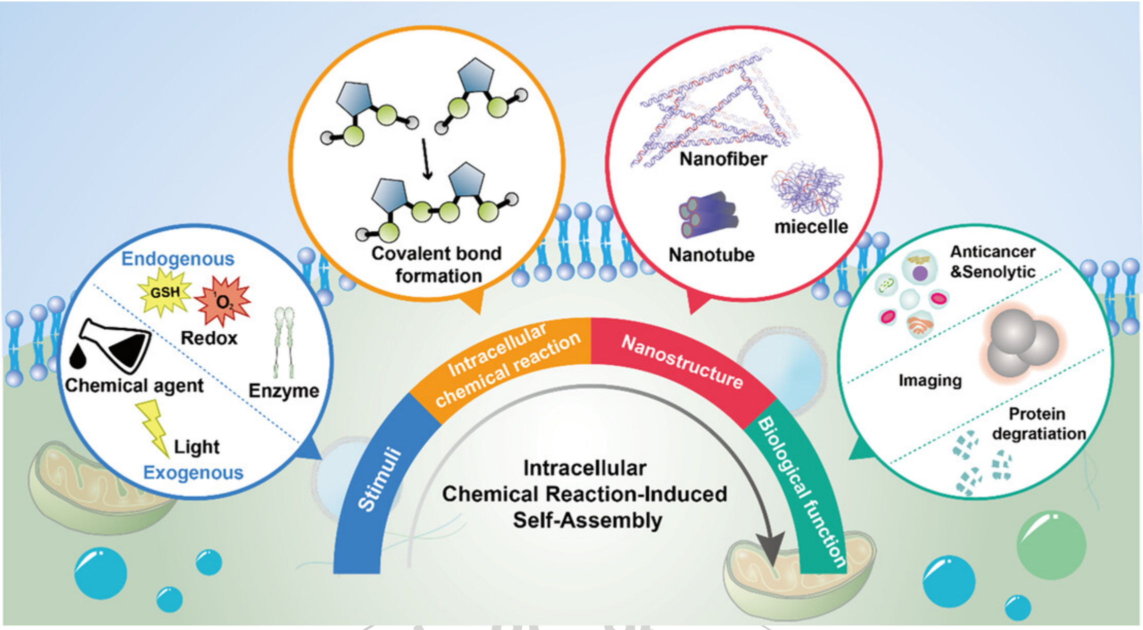
Chair: Kyoung Taek Kim (Seoul National University)

Intracellular Chemical Reaction-Induced Self-Assembly to Control Cellular Fate

Ja-Hyoung Ryu

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

Intracellular assemblies are essential for maintaining cellular functions through interactions mediated by structural recognition. The introduction of artificial structures has attracted significant interest in adjusting cellular functions by interacting with biomacromolecules through activation/inhibition mechanisms. Intracellular chemical-reaction-induced self-assembly has emerged as a promising strategy for creating nanostructures in situ with biofunctionalities for interacting with biomacromolecules. This approach addresses the challenge of synthetic reactions occurring in complex intracellular environments by using various chemical reactions that respond to internal and external stimuli. Recently, we reported that in-situ disulfide polymerization inside mitochondria was achieved through a combination of a large accumulation of monomers (increased local concentration for polymerization) and a high ROS environment (chemical fuel for disulfide reaction). This polymerization process, which occurs in a mitochondrial reducing environment, is autocatalytic and continuously generates ROS while constructing bulky structures that cause mitochondrial dysfunction. This polymerization process is rare inside cells due to the intracellular reductive environment. However, the polymerization process of a thiol-containing monomer further increases the ROS level inside the mitochondria, thereby accelerating the autocatalytic process and inducing mitochondrial dysfunction. This in-situ polymerization shows great potential for anticancer treatment against various cancer cell lines, including drug-resistant cancer cells.


Covalent bond formation
Nanofiber
miecelle
Nanotube
Endogenous
GSH
$^1O_2$
Redox
Chemical agent
Enzyme
Light
Exogenous
Anticancer &Senolytic
Imaging
Protein degratiation
Intracellular chemical reaction
Nanostructure
Stimuli
Biological function
Intracellular Chemical Reaction-Induced Self-Assembly

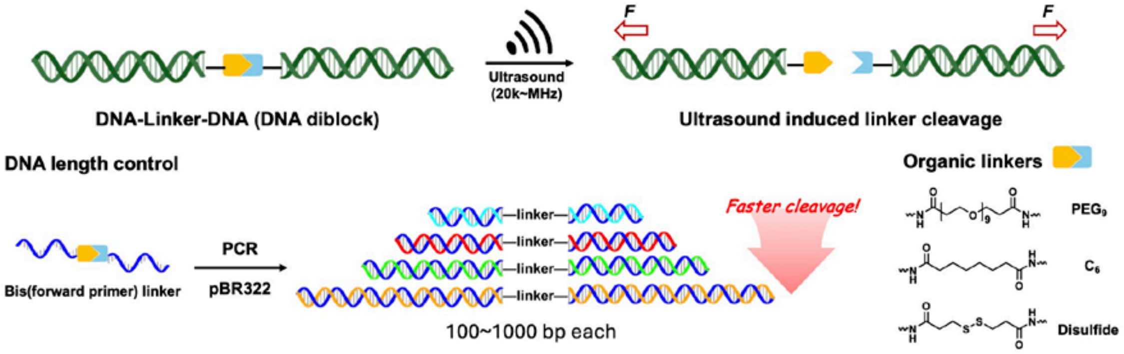
Symposium : **POLY2-4**
Special Symposium by Mid-Career Polymer Chemists
Room 303 FRI 10:15
Chair: Kyoung Taek Kim (Seoul National University)

Fast and precise ultrasound-induced scission of covalent linker within diblock DNA architectures

Minseok Kwak

Department of Chemistry, Pukyong National University, Korea

An ultrasound-induced bond cleavage on mechanopore, a weak bond along the polymer chains, is one of the main foci of polymer mechanochemistry. To date, there are not many studies on the role of polymers, which are mechanical force carriers. Here we report precisely prepared DNAs as the mechanocarriers (MCs) instead of conventional polymers for the mechanochemical bond scission. For this study, a DNA-linker-DNA structure was designed in which a linker is located at the center and two DNA MCs are connected to both termini. We mainly used polymerase chain reaction to engineer DNA MCs and ultrasound as the mechanical force in aqueous media. The effect of DNA MCs was evaluated by changing the length, rigidity, and shape of DNA segments. We investigated to precisely control the bond scission by external force transmitted to the linker through DNA MCs.



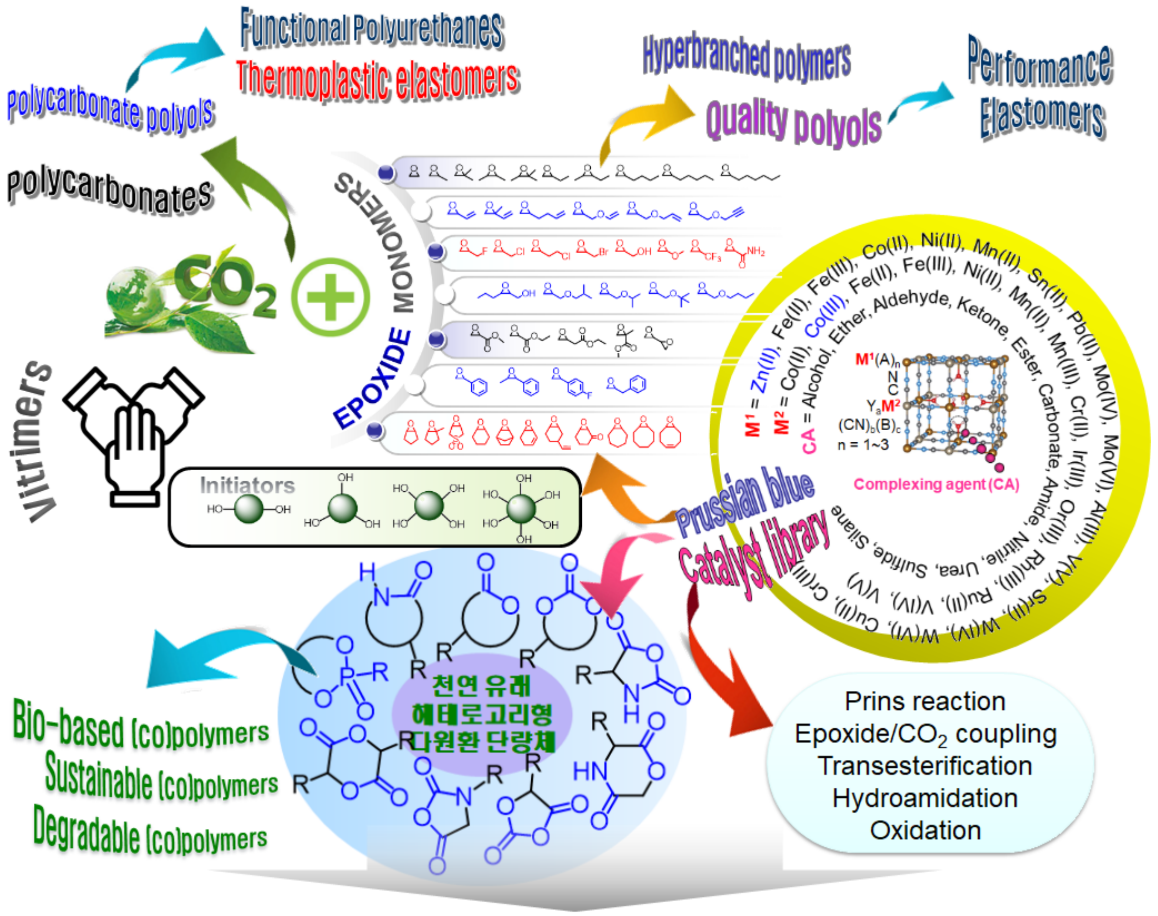
Symposium : **POLY3-1**
Recent Trends in Polymer Synthesis
Room 303 FRI 14:30
Chair: Beom-Goo Kang (Soongsil University)

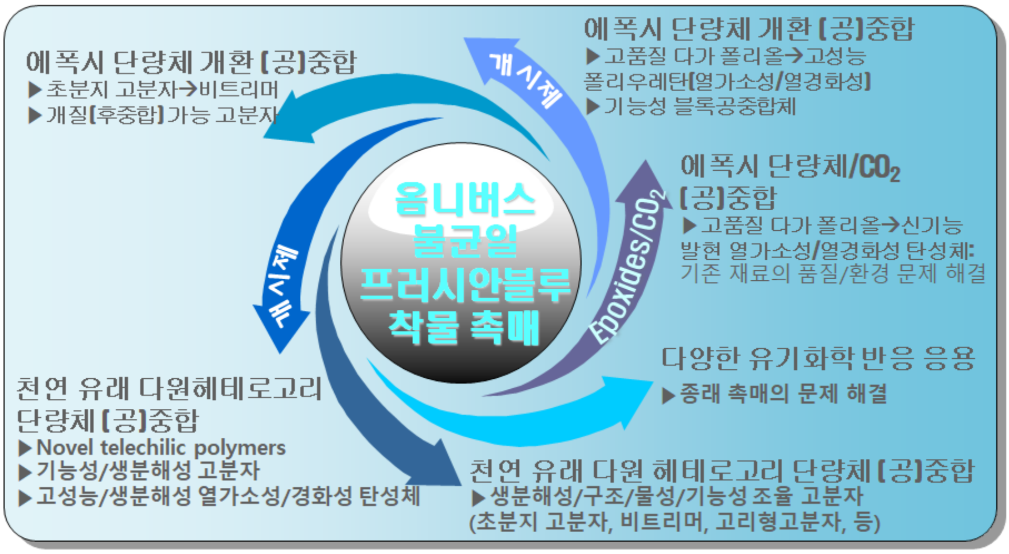
Omnibus Heterogeneous Prussian Blue Complex Catalysts for Ring-opening Polymerizations

Il Kim

Department of Polymer Engineering, Pusan National University, Korea

In order to overcome the specificity of the catalyst, Prussian blue (PB) complex libraries were synthesized as one type of heterogeneous catalyst. By using this method and applying it to the homopolymerization and copolymerization of various types of cyclic monomers, it is possible to solve the conventional fatal problem of using different catalysts (mainly homogeneous catalysts) for each monomer, thereby opening the way for the mass production of ring-opened polymers of various structures that were not possible in the past (Figure 1). By using various epoxy monomers as well as sustainable (biological-derived) polycyclic heterocyclic monomers with initiators with different functionalities, various polymers and terminal substitution polyols (telechelic polymers) were prepared with one type of highly active catalyst. In addition, by using it as a soft segment, we have prepared a thermoplastic/thermoset elastomer that can solve the existing material quality problem that shows performance that is not feasible with conventional catalyst technology. In particular, polymers manufactured using naturally derived monomers are biodegradable, so they can solve social problems caused by plastic waste.





에폭시 단량체 개환 (공)중합
- ▶초분지 고분자→비트리머
- ▶개질(후중합)가능 고분자

에폭시 단량체 개환 (공)중합
- ▶고품질 다가 폴리올→고성능 폴리우레탄(열가소성/열경화성)
- ▶기능성 블록공중합체

에폭시 단량체/CO_2 (공)중합
- ▶고품질 다가 폴리올→신기능 발현 열가소성/열경화성 탄성체: 기존 재료의 품질/환경 문제 해결

다양한 유기화학 반응 응용
- ▶종래 촉매의 문제 해결

천연 유래 다원헤테로고리 단량체 (공)중합
- ▶Novel telechilic polymers
- ▶기능성/생분해성 고분자
- ▶고성능/생분해성 열가소성/경화성 탄성체

천연 유래 다원 헤테로고리 단량체 (공)중합
- ▶생분해성/구조/물성/기능성 조율 고분자 (초분지 고분자, 비트리머, 고리형고분자, 등)

Symposium : **POLY3-2**

Recent Trends in Polymer Synthesis

Room 303 FRI 14:55

Chair: Beom-Goo Kang (Soongsil University)

Synthesis and Self-assembly of Bottlebrush Copolymers into Nanostructured Colloids under Emulsion Confinement

Jaeman Shin

Materials Science and Engineering, Soongsil University, Korea

Hierarchically structured polymeric colloids with controlled shape and morphology have shown great promise for diverse applications. Recently, self-assembly of bottlebrush copolymers received great attention due to their distinct chain architecture with densely grafted side-chains. Herein, rapid production of nanostructured colloids is demonstrated by confined self-assembly of bottlebrush random copolymers (BRCPs) in evaporative emulsion. By quickly evaporating the solvent, symmetric BRCPs with polystyrene (PS) and poly(dimethyl siloxane) (PDMS) side-chains assembled into onion-like particles within 10 minutes. Formation kinetics revealed that particle morphologies were developed instantaneously due to the confinement effect and the BRCP architecture. Furthermore, the tunability of the domain spacings was demonstrated by controlling the degree of polymerization of the side-chains. In an attempt to expand the scope of rapidly accessible particle structures, various morphologies such as concentric lamellae, coiled-cylinders, and spheres-in-spheres were achieved as well as compartmentalized Janus-onion colloids.

Symposium : **POLY3-3**
Recent Trends in Polymer Synthesis
Room 303 FRI 15:20
Chair: Beom-Goo Kang (Soongsil University)

Depolymerization impacts de-bondable polymer adhesives

Hyungwoo Kim

School of polymer science and engineering, Chonnam National University, Korea

This presentation introduces an innovative approach to designing polymer adhesives that can be easily removed when required. We present two categories of thermosetting materials designed for this purpose, each incorporating newly developed deep eutectic solvent (DES) and self-immolative poly(benzyl ether) (PBE). The first type is a photo-curable material that can be processed without solvents, showing comparable adhesion strength to commercial adhesives but can be easily detached upon specific stimuli. The second type is a pressure-sensitive adhesive containing PBE grafts that offer multiple reversible cross-linking points and autonomously depolymerize, making the adhesive both reusable and detachable when no longer necessary. Our design concept holds significant potential for creating functional polymeric materials that simplify end-of-use processes.

Symposium : **POLY3-4**

Recent Trends in Polymer Synthesis

Room 303 FRI 15:45

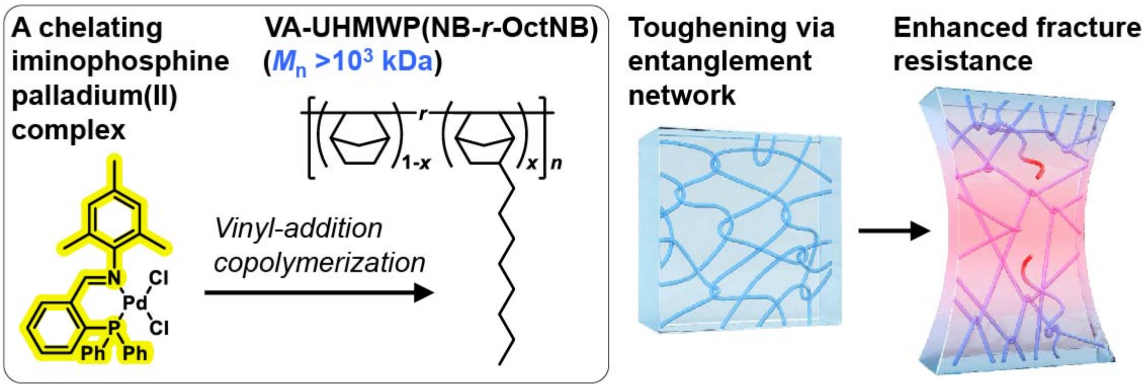
Chair: Beom-Goo Kang (Soongsil University)

An Old Catalyst System Creating a Vinyl-Addition-Type Ultrahigh-Molecular-Weight Polynorbornene Copolymer with Enhanced Fracture Resistance

Chang-Geun Chae

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

The fracture resistance of a cyclic olefin copolymer (COC) was enhanced by incorporating an entanglement network. A vinyl-addition-type ultrahigh-molecular-weight cyclic olefin copolymer (VA-UHMWCOC) with number-average molecular weight (Mn) over 1000 kDa was synthesized by palladium(II)-catalyzed vinyl-addition copolymerization of norbornene (NB) and 5-octyl-2-norbornene (OctNB). Pd(MesN═CHC6H4PPh2)Cl2-based catalyst system produced an active site with optimal electrophilicity, high stability, and highly open geometry. These catalyst properties were often perceived as drawbacks that promote chain transfer through β-hydride elimination in ethylene polymerization, but were advantageous for achieving successive turnover for NB and OctNB owing to the resistance of both two monomers to chain transfer. Consequently, this catalyst system successfully produced vinyl-addition ultrahigh-molecular-weight poly(norbornene-random-5-octyl-2-norbornene) (VA-UHMWP(NB-r-OctNB)) with Mn of >1000 kDa. Employment of 1-hexene as a chain transfer agent in this catalyst system enabled a wide Mn control for VA-P(NB-r-OctNB). Leveraging this control, we enhanced the tensile toughness of VA-P(NB-r-OctNB) by preparing a UHMW analog. This work provides insights into the significance of entanglement network formation for decoupling the stiffness and brittleness of a COC. The introduction of entanglement networks is expected to redefine the traditional structure–property relationships of conventional COCs, thereby providing possibilities for new practical applications.


A chelating iminophosphine palladium(II) complex
N
Pd
Cl
Cl
P
Ph
Ph
Vinyl-addition copolymerization
VA-UHMWP(NB-r-OctNB)
(Mn >10³ kDa)
r
1-x
x
n
Toughening via entanglement network
Enhanced fracture resistance

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

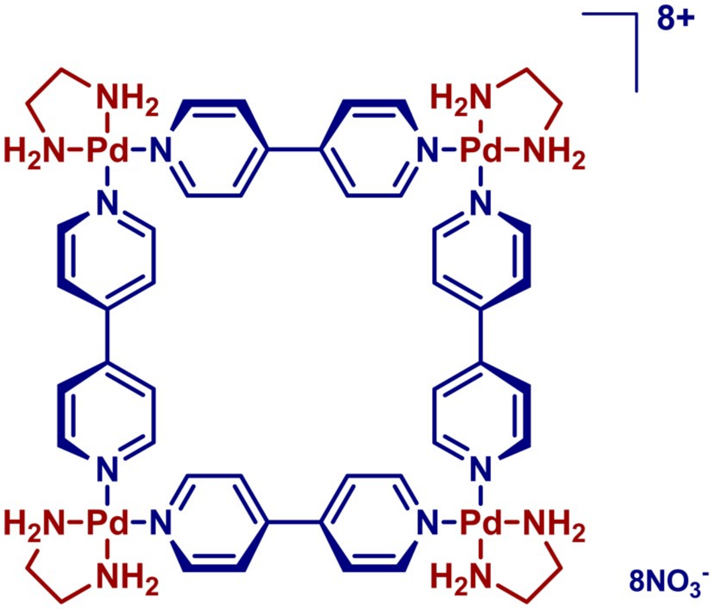
Symposium : **INOR1-1**
Frontiers in Supramolecular and Inorganic Chemistry
Room 405+406 THU 15:40
Chair: Hyo Jae Yoon (Korea University)

Coordination Self-Assembly: From Origins to the Latest Advances

Makoto Fujita

Tokyo College, Institute for Advanced Studies, The University of Tokyo/Division of Advanced Molecular Science, Institute for Molecular Science, Japan

Over the last three decades, our group has been developing a novel construction principle known as "coordination self-assembly." This approach results in the spontaneous formation of diverse structures, including cyclic structures, catenanes, and three-dimensional cages. These assemblies are crafted from numerous transition metal centers and simple coordinating organic molecules. A Pd(II)-cornered square complex marked the inception of coordination assembly, generating not only frameworks but also distinct "spaces" – promising platforms for novel properties and functions. The resulting cages can be vast, acting as large molecular containers that unveil unique chemical properties and reactivity in entrapped substrates. In 1994, the same principle was employed to create an infinite coordination network, demonstrating molecular inclusion within the cavity. Recently, a groundbreaking single-crystal-to-single-crystal guest-exchange phenomenon observed in the porous coordination network has introduced a revolutionary method for determining X-ray structures of small molecules encapsulated in the crystalline self-assembled cages.


8+
8NO$_3^-$

Symposium : **INOR1-2**
Frontiers in Supramolecular and Inorganic Chemistry
Room 405+406 THU 16:10
Chair: Hyo Jae Yoon (Korea University)

Designer Nanomachines for Biological Systems

Jinwoo Cheon

Department of Chemistry, Yonsei University, Korea

One of the important trends of next-generation biomedical sciences is the development of new tools that can accurately image, identify, and execute desired missions in a selectively programmed manner for biological systems. In this talk, I will discuss the design of nanomachines as platform tools for a variety of functionalities such as sensing targeting and signaling of cells and live animals in a selective and efficient way. These tools serve not only as a contrast agent for highly accurate MR imaging but also a modulator for cell signaling of neurons via magneto-genetics for the behavior control of live animals. This is a new approach of controlling neurons via magnetism which will serve for deep brain stimulations via remote and wireless neuromodulations.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **INOR1-3**
Frontiers in Supramolecular and Inorganic Chemistry
Room 405+406 THU 16:40
Chair: Hyo Jae Yoon (Korea University)

Dynamic Capsule Assembly; Stereodivergence in Macrocycle Formation

Myongsoo Lee

Department of Chemistry, Fudan University, China

The precise control of stereoselectivity has been one of the central goals in synthetic chemistry due to the wide appearance of chiral molecules in natural products and pharmaceuticals. Despite remarkable advances, the control of relative and absolute configurations of multiple chirality in macrocyclization is a formidable challenge. Ideally, dynamic chiral confinement of substrates would solve this challenge by switching chirality using readily available physical forces. Here, we show that switchable capsule assembly can be used to reversibly control the chirality of the internal space in which a chiral macrocyclization takes place under chiral confinement, thus confined macrocyclization in a dynamic capsule assembly allows access to any given diastereomers of a macrocycle bearing multiple chirality using external forces. In this presentation, I will show our recent discovery that the chiral capsule entrapping the linear substrate for SNAr macrocyclization can be collectively switchable in their chirality to stereoselectively produce one of four possible diastereomeric macrocycles in a sequential one- pot operation by the addition of hydride and then base to the capsule solution (Scheme).
Scheme; Stereodivergent Macrocyclization in Switchable Capsule

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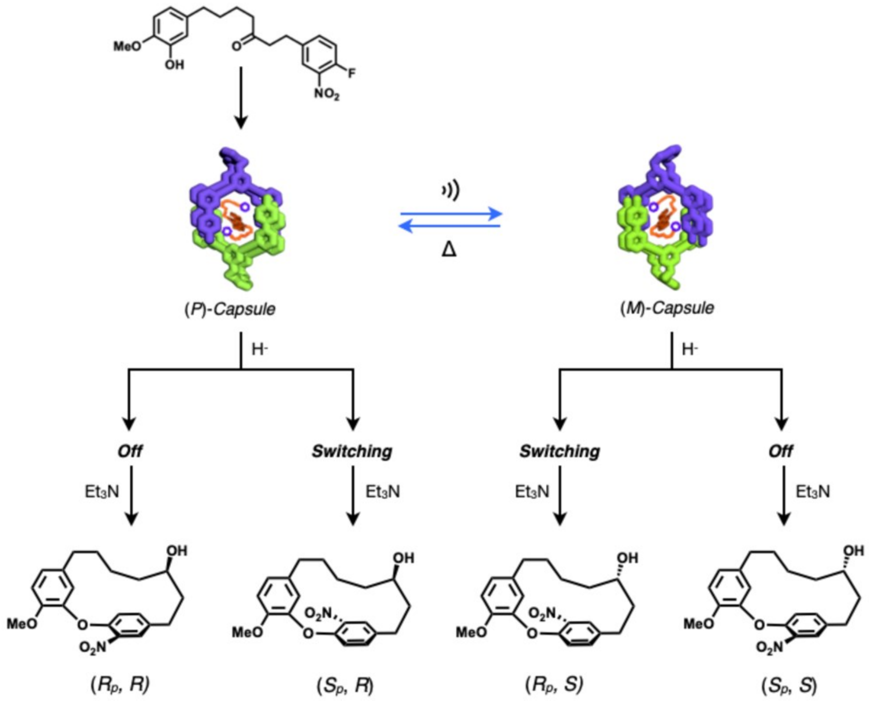
MeO
OH
O
F
NO2
))
Δ
(P)-Capsule
(M)-Capsule
H-
H-
Off
Switching
Switching
Off
Et3N
Et3N
Et3N
Et3N
OH
MeO
O
O2N
(Rp, R)
(Sp, R)
(Rp, S)
(Sp, S)

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **INOR1-4**
Frontiers in Supramolecular and Inorganic Chemistry
Room 405+406 THU 17:10
Chair: Hyo Jae Yoon (Korea University)

A truly professional chemist who always explores new pathways

Eunsung Lee

Department of Chemistry, Seoul National University, Korea

Professor Kimoon Kim stands as a paragon of true professionalism within chemistry. Renowned as a pioneer in supramolecular chemistry, asymmetric MOF, and 2D organic materials, his career has been characterized by an unyielding commitment to exploring new pathways in these cutting-edge domains. His groundbreaking contributions have left an indelible mark on the scientific community, shaping the landscape of modern chemistry. In addition to his influential work in established fields, Prof. Kim has recently ventured into the emerging realm of sound chemistry, showcasing his versatility and forward-thinking approach. This diversification underscores his dedication to staying at the forefront of scientific innovation. As a leader in the field, he not only advances knowledge through his groundbreaking research but also inspires the next generation of chemists. Prof. Kim's legacy is one of continual exploration, pushing the boundaries of what is known and setting the stage for the future of chemistry. I will briefly present his amazing career.

Symposium : **INOR1-5**

Frontiers in Supramolecular and Inorganic Chemistry

Room 405+406 THU 17:20

Chair: Hyo Jae Yoon (Korea University)

My journey to supramolecular chemistry

Kimoon Kim

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

My journey into the realm of supramolecular chemistry began with a serendipitous encounter with cucurbituril, a molecule resembling a hollow pumpkin, in a library. This initial fascination led us to the discovery and isolation of other members of the host family, opening new avenues in supramolecular chemistry. My love affair with the host family for more than three decades has yielded extensive fundamental studies and applications including imaging, isolation, and purification of proteins. My curiosity about porous materials directed us towards the synthesis of metal-organic frameworks (MOFs), exemplified by POST-1, alongside organic porous materials like porphyrin boxes, and polymer nanocapsules. The development of highly conducting two-dimensional polymers (C2Ps) marks the latest chapter in our quest for innovative materials. Moreover, I have always been keen on exploring novel scientific avenues; a recent endeavor involves harnessing audible sound to control chemical reactions in a spatiotemporal manner. This journey has been not only immensely rewarding but also profoundly enjoyable.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **INOR2-1**
Recent Trends in Organometallic Materials Chemistry
Room 405+406 FRI 09:00
Chair: Kang Mun Lee (Kangwon National University)

Exploring Photoactivities of Au(I) Complexes

Youngmin You

Chemical and Biomolecular Engineering, Yonsei University, Korea

Linear, heteroleptic Au(I) complexes produce long-lived fluorescence with negligible contributions of prompt fluorescence, primarily due to a rapid equilibrium between their singlet and triplet states. This efficient spin mixing provides a unique principle for creating high-efficiency, roll-off-free hyperfluorescence electroluminescence devices. To maximize the utility of electroluminescence, my group investigated factors that control radiative and nonradiative processes in excited-state Au complexes. Our mechanistic studies revealed the key role of the d-orbital of the Au center, despite its d10 electronic configuration. This discovery enabled the highest efficiency electroluminescence in the near-infrared regions from Au(I) complex emitters. The less electron-demanding, low-valent Au(I) center also imparts strong photoreducing power to the complexes. The Au(I) complex, having the 1,3-diphenylbenzo[d]imidazolium-based carbene ligand and the 1,3,6,8-tetramethylcarbazolide ligand, exhibits an excited-state oxidation potential as cathodic as -2.16 V vs SCE in DMSO, making it capable of reducing redox-resistant aryl chloride substrates for C-C cross-coupling reactions.

Symposium : **INOR2-2**
Recent Trends in Organometallic Materials Chemistry
Room 405+406 FRI 09:25
Chair: Kang Mun Lee (Kangwon National University)

Development of Organic Phosphorescent Materials for OLED Display

Yun Hi Kim

Department of Chemistry, Gyeongsang National University, Korea

Organic light-emitting diodes (OLEDs) have been utilized for several applications in various displays over the past 25 years. The current OLED display technology is aiming to develop devices with higher efficiency and a longer lifetime, but it remains elusive. The phosphorescent red and green-based devices have been successfully commercialized in the market due to their better efficiency and long lifetime. However, in the case of blue OLED, it is still utilizing only low-efficiency fluorescent materials because of the short device lifetime of phosphorescent and thermally activated delayed fluorescence (TADF) OLEDs. Much research is still being done to find ways to extend the lifetime of blue phosphorescent.In this presentation, I will introduce the molecular design of organic phosphorescent materials for OLED display.

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Symposium : **INOR2-3**
Recent Trends in Organometallic Materials Chemistry
Room 405+406 FRI 09:50
Chair: Kang Mun Lee (Kangwon National University)

Earth-abundant Transition Metal Luminophores

Yoonsu Park

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

Molecular luminescent compounds play a pivotal role in various industrial applications, particularly in the development of light-emitting devices. Common strategies for enhancing emission efficiency and excited-state lifetime often involve the utilization of 2nd or 3rd-row transition metal complexes to achieve phosphorescent emission via facile intersystem crossing (ISC), or organic chromophores exhibiting thermally-activated delayed fluorescence. Despite notable successes, challenges persist, including the scarcity of rare-earth elements like iridium or platinum, and the limited tunability of organic chromophores. In this study, we introduce a novel class of earth-abundant transition metal luminophores designed to address these challenges. Through rational ligand design, we have successfully mitigated issues associated with rapid relaxation from the excited state and slow ISC. This design strategy has led to the realization of vibrant green/blue emission with a remarkably high quantum yield exceeding 50%. Characterization of our luminophores utilizing a time-correlated single photon counting technique revealed a lifetime of the emissive state exceeding hundreds of nanoseconds. Transient absorption analysis confirmed the presence of excited-state absorption features, providing further insights into the excited-state dynamics. Furthermore, the excited-state energy of our luminophores has been leveraged for energy transfer catalysis. We demonstrated the catalytic isomerization of a substrate possessing >60 kcal/mol of triplet energy upon irradiation, showcasing the potential applications of our compounds in energy transfer processes.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **INOR2-4**

Recent Trends in Organometallic Materials Chemistry

Room 405+406 FRI 10:15

Chair: Kang Mun Lee (Kangwon National University)

Bioinspired Metal-Ligand Cooperative Transformation of Small Molecule

Yunho Lee

Department of Chemistry, Seoul National University, Korea

Several metalloenzymes employ the metal-ligand cooperativity, in particular with the first-row transition metal ion and amino acid residues in their active site for processing biologically important chemical transformations of small molecules such as H2, COx and NOx. Inspired by such M-L cooperative reactions, we employ metal-ligand cooperation (MLC) as a novel synthetic methodology to expand the role of transition metals in small molecule conversion. While non-innocent phosphide and silyl ligands are relatively rare, our group works with a new type of metal-ligand cooperation by using an anionic PPP pincer type ligand. The central phosphide moiety can act as a 1 or 2 electron donor, which was recognized from the studies of various nickel and cobalt complexes. The MLC redox chemistry of a (PPP)M scaffold (M = Ni or Co) and its application in C1 conversion will be presented. Both nickel and cobalt complexes reveal the reversible formation of a P–P bond involving a single electron exchange between metal and P. By using this reversible conversion, a synthetic cycle for isocyanate generation starting from the nickel amide species was successfully accomplished. Various bond activations are achieved at the M-P-P-M site, which is equivalent to the metal-phosphinyl radical operating as an active MLC site. In particular, a (PPP)Co scaffold reveals a unique azide coordination to give a phosphazide cobalt species. Its redox property and MLC transformation will be discussed.

Symposium : **INOR2-5**

Recent Trends in Organometallic Materials Chemistry

Room 405+406 FRI 10:40

Chair: Kang Mun Lee (Kangwon National University)

Syntheses, Structures, and Optical Properties of Homochiral Organic-Inorganic Hybrid Materials

Kang Min Ok

Department of Chemistry, Sogang University, Korea

Crystalline materials with noncentrosymmetric (NCS) structures have garnered significant interest in the industry attributed to their inherent properties such as piezoelectricity, ferroelectricity, and second-harmonic generation (SHG). While inducing NCS structures using asymmetric building units remains a challenge, this presentation explores a novel approach employing homochiral organic molecules for the systematic and efficient synthesis of such materials. Specifically, the talk aims to provide a comprehensive overview of the synthesis, structure determination, and multifaceted optical properties of these homochiral materials.The synthesis focuses on a series of homochiral organic-inorganic hybrid materials, utilizing chiral organic templates. The crystal structures, determined by single crystal X-ray diffraction, reveal homochiral materials with chiral space groups, highlighting the uniqueness of the structural arrangement facilitated by the chiral structure-directing materials. Intermolecular interactions, including hydrogen bonds and π-π stacking, contribute to the robust formation of frameworks. The presented NCS compounds demonstrate interesting linear and nonlinear optical properties, exhibiting efficient photoluminescence over a broad visible spectrum as well as SHG. The unique phenomena stem from the chiral centers in organic templates within NCS environment, adding a new dimension to the exploration of optical properties.

Symposium : **INOR3-1**
Recent Trends in 2D Inorganic Materials
Room 405+406 FRI 14:30
Chair: Intek Song (Andong National University)

Porous organic polymers for gas separation, conductivity, and catalysis

Chang Seop Hong

Department of Chemistry, Korea University, Korea

Porous Organic Polymers (POPs) are organic networks linked by covalent bonds, showcasing diverse applications such as the selective capture and separation of specific gases, ion conductivity, and catalysis. These POPs, characterized by robust structures, exhibit exceptional long-term stability while maintaining high performance. The capability of POPs in capturing and purifying crucial industrial gases is enhanced by adjusting pore size and properties through postsynthetic methods that introduce targeted functional groups onto the pore walls. Our research focuses on leveraging the unique pore characteristics of POPs to efficiently separate key industrial gases, enhance ion conductivity, and optimize catalytic reactions. In this presentation, I will discuss our synthetic strategies for POP functionalization and highlight the intriguing properties that result from these modifications.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **INOR3-2**

Recent Trends in 2D Inorganic Materials

Room 405+406 FRI 15:00

Chair: Intek Song (Andong National University)

Surface Engineering of Pt Based Ultrathin Nanosheets for Boosting Electrocatalytic Oxygen Reduction Reaction

Jong Wook Hong

Chemistry, University of Ulsan, Korea

Ultrathin two-dimensional (2D) metal nanosheets have been the subject of intensive research for various catalytic reactions due to their unique properties coming from anisotropic structures and atomic thickness compared with bulk. Ultrathin metal nanosheets with high surface-to-volume ratio significantly enhanced the catalytic performances via their high utilization efficiency of the metal. In addition, the development of bimetallic alloy nanosheets has provided a route to improve the desirable properties for various electrocatalytic reactions in comparison to monometallic nanosheets. Herein, we present a rational synthetic approach mediated by sequential kinetic-thermodynamic metal reduction control for holey ultrathin Pt3M alloy nanosheets (Pt3M HU-NSs, where M = Ni, Co, Cu, Ir, Pd, Ru, Rh, Fe, and Mn) with a thickness of approximately 3 nm and abundant edge sites. The unique sequential kinetic-thermodynamic metal reduction control provides fine-tuning over the anisotropic 2D growth of Pt-based alloy nanostructures by restraining the three-dimensional growth of metals and stabilizing low coordinated edge sites. The Pt3Ni HU-NSs display significantly enhanced oxygen reduction reaction activity and stability compared to other Pt3M HU-NSs, pure Pt HU-NSs, and the state-of-the-art Pt/C catalysts, attributed to their distinctive morphology and composition. In addition, B-incorporated Pt3M HU-NSs exhibited dramatic improvement in ORR performance. We believe that this synthesis strategy provides insights into the development of ultrathin 2D metal structures with abundant edge sites that can be deployed to create advanced electrocatalysts.

Symposium : **INOR3-3**
Recent Trends in 2D Inorganic Materials
Room 405+406 FRI 15:25
Chair: Intek Song (Andong National University)

Synthesis and chemical modulation of MXenes for electronic applications

Seon Joon Kim

Materials Architecturing Research Center, Korea Institute of Science and Technology, Korea

MXenes are a rising family of two-dimensional (2D) transitional metal carbides/nitrides with high electrical conductivity and a high density of surface functionalities. These unique properties allow MXenes to perform in areas where conventional materials have been unable to reach. Another large advantage of MXenes is the large tunability in their physicochemical properties. For example, chemical properties can be modified by synthesizing MXenes with different transition metals or transforming the intrinsic surface functional groups into diverse chemical moieties. Also, as MXenes are structurally anisotropic 2D sheets, their electrical properties can be further tuned by modulating the assembly or alignment of individual sheets. In this talk, versatile methods to efficiently modulate the chemical properties and structure of MXenes will be discussed. Also, strategies to utilize these techniques into fabricating nanocomposites and electronic applications will be discussed.

Symposium : **INOR3-4**

Recent Trends in 2D Inorganic Materials

Room 405+406 FRI 15:50

Chair: Intek Song (Andong National University)

Heterointerface engineering of 2D nanoplates for highly efficient electrocatalysts

Jongsik Park

Department of Chemistry, Kyonggi University, Korea

The development of highly efficient electrocatalysts has been investigated for sustainable and clean hydrogen production. Heterointerface engineering of juxtaposed different material phases can greatly modify the electronic structure of the catalyst, resulting to increase the catalytic activity and stability. Herein, we suggest the synthetic methodologies how to rationally design the heterointerface within the 2D nanoplates via cation exchange reaction. The multiphasic hetero-nanostructures with modulated lattice parameters will provide new synthetic methodologies for the design and synthesis of nanocatalysts with novel physicochemical properties.

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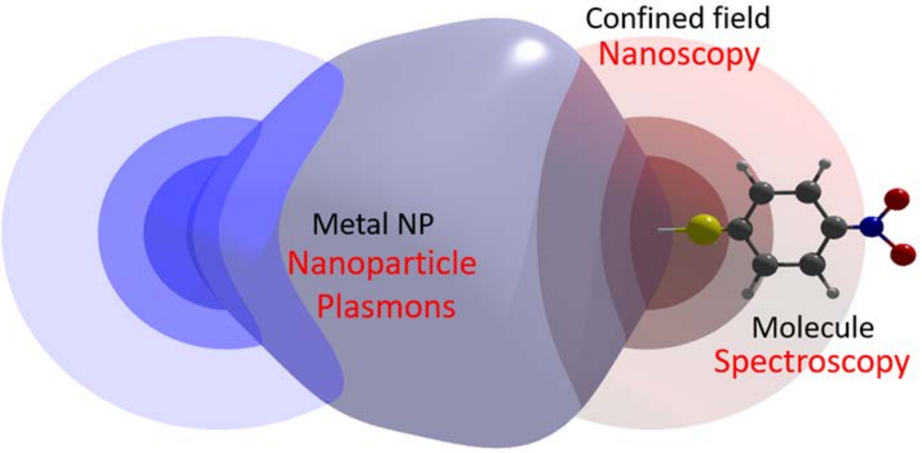
Award Lecture in Division : **PHYS1-1**
Physical Chemistry of Life
Room 401+402 THU 15:40
Chair: Sang-Hee Shim (Korea University)

Nano-plasmonics for single-molecule spectroscopy, imaging and photo-catalysis

Zee Hwan Kim

Department of Chemistry, Seoul National University, Korea

Photoexcitation of noble metal nanostructures leads to the coupled oscillation of confined light-field and conduction electrons, which is called the localized surface plasmons. My research group is developing new ways to utilize the plasmons and field confinement to do new molecular spectroscopy and imaging, and spectroscopically studying the underlying mechanism of unusual photochemistry induced by plasmons. My talk will specifically focus on the most recent results from my group, which include the plasmon-induced non-thermal vibrational excitation, 2nd-order nonlinear optical mixing, the enhancement of light emission from electrically biased molecular tunnel junctions, and the nanoscale mid-IR imaging of the structure and chemistry of few-layer graphene.


Confined field
Nanoscopy
Metal NP
Nanoparticle
Plasmons
Molecule
Spectroscopy

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **PHYS1-2**
Physical Chemistry of Life
Room 401+402 THU 16:10
Chair: Sang-Hee Shim (Korea University)

Cellular Tunneling Nanotubes

Jong-Bong Lee

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

Tunneling nanotubes (TNT) serve as a novel conduit for long-range intercellular communication, bridging cells over considerable distances spanning several cell diameters. Despite their delicate structure, capable of persisting for extended durations, the mechanisms underlying their expansion and resilience remain elusive. Through the meticulous examination of the spatiotemporal dynamics of TNT formation, derived from filopodial bridges known as two-filopodia complexes (DFB), we have uncovered the pivotal role played by the helical architecture of DFB in facilitating the transition to TNT. Notably, the termination of TNTs establishes contact with the recipient cell's surface through cadherin-cadherin adhesion, fostering a tight intercellular connection. Our investigations confirmed the transfer of Ca2+ ions between cells via TNTs, while discernibly nanoparticles exhibit restricted passage. This observation supports the notion of TNTs predominantly manifesting as closed-ended structures. Intriguingly, we observe nanoparticle migration between cells through TNTs only in the absence of N-cadherin clusters at their terminal. These findings provide compelling insights into the potential mechanisms governing cellular material transport through TNTs, a phenomenon I will elucidate further in my presentation.

Symposium : **PHYS1-3**

Physical Chemistry of Life

Room 401+402 THU 16:35

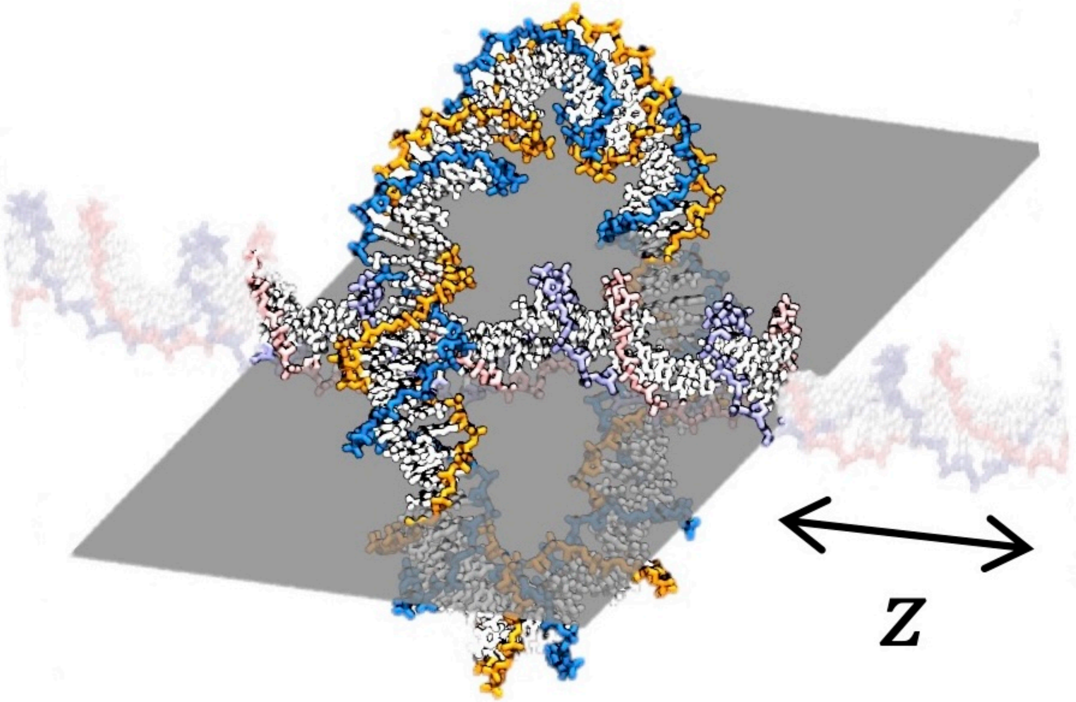
Chair: Sang-Hee Shim (Korea University)

Understanding the structure and dynamics of small circular DNA molecules by molecular simulations

Yeonho Song, Jun Soo Kim[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

In cellular environments, the intricate folding of DNA plays a pivotal role in its structural and functional integrity. To emulate the pronounced curvatures characteristic of intracellular DNA, sub-100 base pair (bp) DNA minicircles have been utilized as models for sharply bent DNA configurations. Here, we present extensive molecular dynamics (MD) simulations of double-stranded DNA minicircles with lengths below ~100 base pairs (bp), focusing on the elucidation of the structural and dynamic properties of the DNA double helix subject to severe bending. In particular, we discuss the sequence-dependent coupling between twist and bending and its implications in nucleosome formation. Furthermore, this research explores the structural dynamics of circular DNA within mechanically interlocked architectures, namely rotaxanes and catenanes, evaluating their potential application in the realm of nanoscale devices. Our findings indicate that the inherent stiffness and precise geometry of small circular DNA enable their robust translational and rotational movements on a linear DNA axle within a DNA rotaxane framework. The insights from our studies serve as a foundation for designing DNA-based nanoscale devices.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Symposium : **PHYS1-4**
Physical Chemistry of Life
Room 401+402 THU 17:00
Chair: Sang-Hee Shim (Korea University)

Precise Gene Editing in Genetic Diseases

Sangsu Bae

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

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

Symposium : **PHYS1-5**
Physical Chemistry of Life
Room 401+402 THU 17:25
Chair: Sang-Hee Shim (Korea University)

Revisiting the stickers-and-spacers framework: what does an IDR do in biomolecular phase separation?

Jeong-Mo Choi

Department of Chemistry, Pusan National University, Korea

The stickers-and-spacers framework, proposed in 2018 (Wang *et al*., *Cell* 2018), offers insights into the collective behaviors of heteropolymers, particularly biomolecules such as proteins and nucleic acids. Inspired by the associative polymer theory, this model categorizes polymer constituents into two groups: those engaging in chain-chain interactions (*stickers*) and those that do not (*spacers*). While the model's simplicity has garnered significant interest, it has also sparked misunderstandings and critiques. Notably, the existence of a hierarchy of stickers, depending on their contributions to chain-chain interactions, has been suggested. In this presentation, I will elucidate the framework and its modifications, and present recent findings that offer a non-canonical illustration of the stickers-and-spacers framework.

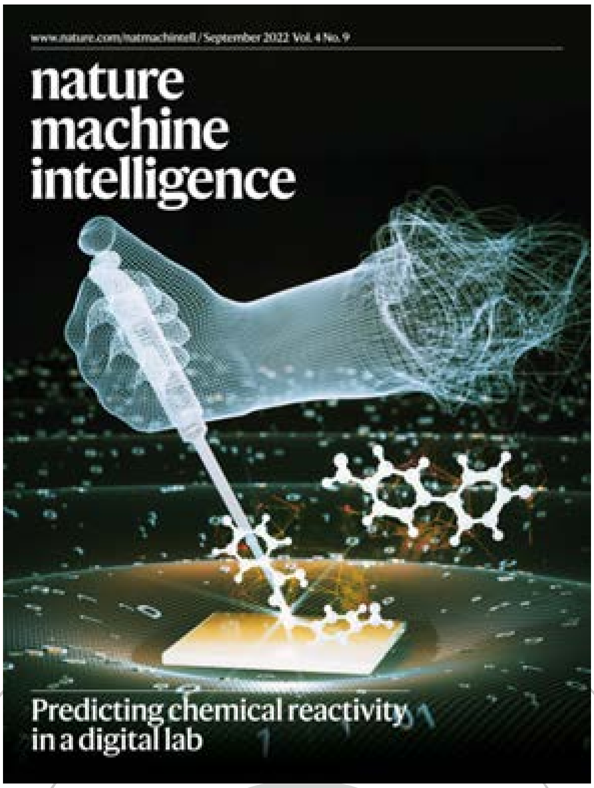
Award Lecture in Division : **PHYS2-1**
New Insights into the Physical Chemistry for Energy and Battery Applications
Room 401+402 FRI 14:30
Chair: Minho Kim (Kyung Hee University)

Synthetic Planning and Predictions Enabled by AI

Yousung Jung

Department of Physical Chemistry, School of Chemical and Biological Engineering, Korea

Reliable prediction of chemical reactivity remains in the realm of knowledgeable synthetic chemists. Automating this process by using artificial intelligence could accelerate synthesis design in future digital laboratories. While several machine learning approaches have demonstrated promising results, most current models use language models which is difficult to interpret and deviate from how human chemists analyze and predict reactions based on electronic changes. In this talk, I will talk about our recent efforts to learn organic reactivity based on chemical rules and algorithms. The issues related to the current reaction datasets and hence the importance of data curation to further improve the models will be discussed. I will then propose a new organic synthesis prediction AI methodology that can predict the reaction mechanisms with various chemical conditions.


www.nature.com/natmachintell / September 2022 Vol. 4 No. 9
nature machine intelligence
Predicting chemical reactivity in a digital lab

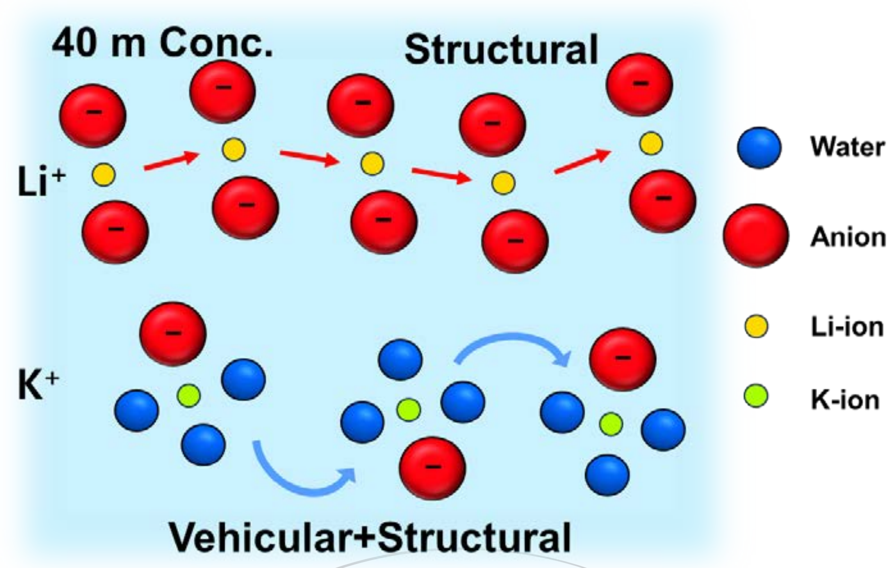
Symposium : **PHYS2-2**
New Insights into the Physical Chemistry for Energy and Battery Applications
Room 401+402 FRI 15:05
Chair: Minho Kim (Kyung Hee University)

Li+ ion transport dynamics in “water-in-salt” electrolytes for aqueous Li ion battery.

Kyungwon Kwak

Department of Chemistry, Korea University, Korea

Electrolytes are ubiquitous and indispensable in all electrochemical devices including electrolytic cells, capacitors, fuel cells, or batteries. Their function is the same in devices for serving as the medium for the ion transport between electrodes. The electrolyte determines how fast the energy could be released by controlling the rate of mass flow within the battery. Thus, it has been suggested that the solvation structures and dynamics of Li ions in liquid electrolyte play an essential role to Li-based battery performance. Lithium ions in highly concentrated aqueous electrolyte used in lithium-ion battery (LIB) shows unexpectedly high ion mobility despite high viscosity of the concentrated electrolyte. Here, carrying out femtosecond IR pump-probe, two-dimensional IR spectroscopy studies, and dielectric relaxation spectroscopy, we show that a considerable amount of water even in highly concentrated electrolyte solutions exhibits bulk-like water properties and forms hydrogen-bonding network structures. Furthermore, time-resolved rotational anisotropy, spectral diffusion dynamics, and molecular dynamics simulations of water indicate the presence of interfacial water on ion aggregate networks that helps reducing electrostatic friction of hydrated lithium ions, resulting in an unexpectedly rapid transport of lithium ions.


40 m Conc.
Structural
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Water
Anion
Li-ion
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Symposium : **PHYS2-3**

New Insights into the Physical Chemistry for Energy and Battery Applications

Room 401+402 FRI 15:30

Chair: Minho Kim (Kyung Hee University)

Exfoliated Nanosheets of Layered Metal Hydroxide as a Long-Lived and Recyclable Oxygen Evolution Electrocatalyst

Jong Hyeon Lee

Department of Chemistry, The Catholic University of Korea, Korea

Extensive research efforts are underway to address the projected surge in global energy needs, driving the quest for renewable energy sources and efficient energy storage systems. Electrochemical water splitting, facilitated by electric power, emerges as a promising way for generating chemical fuels with minimal environmental impact. The oxygen evolution reaction (OER) slows the water splitting because of its sluggish electron-transfer kinetics compared to the hydrogen evolution reaction. Noble-metal-based compounds, such as RuO_2 and IrO_2, are considered the most active OER catalysts; however, their natural scarcity and expensive nature hinder their practical use. This study investigated the electrochemical properties of the monolayer layered metal (Co, Ni, Fe) hydroxide and their thin films for active OER electrocatalysis. We further suggested boron-doped metal hydroxide nanosheets for long-lived and recyclable OER catalysts. First, the nanosheet of cobalt hydroxide was prepared using a liquid exfoliation of anion-containing bulk metal hydroxides, which has positively charged hydroxide layers with expanded interlayer spaces, charge-balancing anions, and water molecules. Then, a wet $NaBH_4$ treatment produced the boron-doped metal hydroxide nanosheets, exhibiting a high OER activity and stability under 1M KOH/0.5M NaCl solution.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **PHYS2-4**

New Insights into the Physical Chemistry for Energy and Battery Applications

Room 401+402 FRI 15:55

Chair: Minho Kim (Kyung Hee University)

First-principles simulations toward semiconductor-based energy devices

Han Seul Kim

Department of Advanced Materials Engineering, Chungbuk National University, Korea

Low-dimensional materials such as two-dimensional materials and crystal materials with internal polyhedral structures attract great attention due to their extraordinary controllability over electrical/optical properties. In this regard, they are expected to be the key materials for various next-generation devices for energy harvesting, energy storing, and energy-efficient semiconductors. In this presentation, several computational studies based on density functional theory (DFT) will be introduced for the application of low-dimensional materials to various semiconductor-based energy devices. In particular, it will be highlighted that the material engineering parameters revealed by electronic structure calculations can act as key components toward seamless collaborations with experiments.References[1] Nano Today 55, 102184 (2024)[2] Adv. Energy. Mater. 14, 2302579 (2024)[3] Adv. Mater. 35, 2301141 (2023)

133rd General Meeting of the Korean Chemical Society
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Award Lecture in Division : **ANAL1-6**
Recent Status in NMR-based Analytical Chemistry
Room 103+104 THU 17:30
Chair: Youngbok Lee (Hanyang University)

Development of multiresidue analysis for prohibited substances in antidoping analysis by liquid chromatography and mass spectrometry: for worldwide sports events

Ki Hun Kim

Analytical Chemistry, Doping Control Center, Korea Institute of Science and Technology, Korea

World Anti-Doping Agency (WADA) requires to the doping laboratory to analyze prohibited substances and their metabolites in various classes and a screening method which can detect multi-substances is an important challenge in the field of doping control. Particularly for global sports events like the Olympics, where numerous samples must be analyzed in a short period, it is very important to integrate various existing analytical methods into a single method to save time, manpower, and resources. In this study, we developed an analytical method that integrates three existing methods: dilute and inject, peptide analysis, and LLE-based analysis. Many drugs excreted in urine exist as metabolites of glucuronide form, and we used the enzyme glucuronidase, which can hydrolyze them to their parent form. We also used a mixed-mode SPE of a weak cation exchange mechanism, to extract peptides and polar substances simultaneously. Furthermore, we introduced a method of diluting the dried samples with the urine to recover specific drug of glucuronide form or polar drugs that are not extracted. We conducted various optimizations and validation for SPE extraction and enzyme reaction efficiency depending on buffer composition, temperature and pH. In particular, we were able to remove matrix interference using a high-resolution mass spectrometer, the orbitrap, and performed high-efficiency analysis of highly polar drugs like meldonium. The developed analytical method can simultaneously analyze over 350 prohibited drugs and their metabolites, and using this method, we successfully performed sample analysis for large-scale sports events like the Pyeongchang Winter Olympics.

Symposium : **ANAL1-1**
Recent Status in NMR-based Analytical Chemistry
Room 103+104 THU 15:40
Chair: Young-Kwan Kim (Dongguk University)

Dynamic Nuclear Polarization: Sensitivity Boost for Magnetic Resonance Spectroscopy and Imaging

Youngbok Lee

Department of Chemical and Molecular Engineering, Hanyang University, Korea

One of the most crucial analytical tools for studying chemistry and biology is magnetic resonance (MR) research. It offers comprehensive details on molecular interactions in addition to the structures of macromolecules and small compounds. Due to the weak Zeeman splitting of the nuclear spin energy states, which causes MR's intrinsic low sensitivity, extended signal averaging times or high spin concentrations are frequently needed. Many techniques have been investigated to raise MR's sensitivity. Specifically, hyperpolarization of the nuclear spins can yield substantial signal increases. In comparison to thermal polarization, the MR signals of hyperpolarized samples are amplified by several orders of magnitude. Dynamic Nuclear Polarization (DNP) is a flexible method that may be used to polarize a wide range of nuclei at low temperatures in the solid state. After a dissolving stage, the method produces a liquid sample that is hyperpolarized. In a variety of scientific domains, including metabolic imaging and enzyme catalysis, extensive information has been obtained thanks to the ensuing signal augmentation. By examining protein-ligand interactions, real-time kinetic and mechanistic research for chemical reactions, and metabolic imaging for early-stage cancer detection, this lecture seeks to expand the applicability of DNP into new fields of chemistry and biology.

Symposium : **ANAL1-2**

Recent Status in NMR-based Analytical Chemistry

Room 103+104 THU 16:00

Chair: Young-Kwan Kim (Dongguk University)

Inhibition of cytotoxicity of pathogenic huntingtin protein by an IP3 receptor fragment

Min-Duk Seo

College of Pharmacy, Ajou University, Korea

Huntington's disease (HD) is caused by abnormally increased CAG repeats in the first exon of Htt gene, which encodes the huntingtin protein (Htt). There is currently no cure for treating HD. To develop strategies for inhibiting HD pathogenesis, the intermolecular interaction of Htt with IP3 receptor 1 (IP3R1) was investigated. We designed the peptide (termed ICT60) corresponding to a coiled-coil motif in the C-terminus of IP3R1. Several biophysical approaches revealed the strong and specific binding of ICT60 to the N-terminal part of the first exon of Htt (HttEx1). ICT60 inhibited not only amyloid formation by HttEx1, but also the cytotoxicity and cell-penetration ability of the amyloid fibrils of HttEx1. We propose a mechanical model explaining how an IP3 receptor-inspired molecule can modulate cytotoxic amyloid formation by Htt, providing a molecular basis for developing therapeutics to treat HD.

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Symposium : **ANAL1-3**
Recent Status in NMR-based Analytical Chemistry
Room 103+104 THU 16:20
Chair: Young-Kwan Kim (Dongguk University)

NMR applications in Energy materials

Heeyong Park

LG Chem, Korea

Rational design of high-performance electrodes necessities a deep understanding of the interplay between surface chemical structure and reactant interactions, and working/degradation mechanisms in energy materials. This talk highlights the power of Nuclear Magnetic Resonance (NMR) spectroscopy as a frontline tool in unveiling this critical information. We will explore the latest and most advanced NMR applications, including DNP-SENS(Surface Enhanced NMR spectroscopy)[1], SCREAM(Specific Cross Relaxation Enhancement by Active Motions)[2]-DNP, NMR dynamics techniques[3] and In-Situ NMR for battery. --------------------------------------References1.Lesage, A. et al. Surface Enhanced NMR Spectroscopy by Dynamic Nuclear Polarization. J. Am Chem. Soc. 44, 15459-15461 (2010) 2.Park H. et al. Heteronuclear cross-relaxation effect modulated by the dynamics of N-functional groups in the solid state under 15N DP-MAS DNP. J. Magn. Reson. 312, 10688 (2020)3.Park H. et al. Insights into Water Interaction at the interface of Nitrogen-Functionalized Hydrothermal Carbons. J. Phys. Chem. C 123, 25146-25156 (2019)

Symposium : **ANAL1-4**
Recent Status in NMR-based Analytical Chemistry
Room 103+104 THU 16:50
Chair: Youngbok Lee (Hanyang University)

NMR-based metabolomic approaches in human disease research

Geum-Sook Hwang

Integrated Metabolomics Research Group, Korea Basic Science Institute, Korea

NMR-based metabolomic approaches have become increasingly valuable in human disease research due to their ability to provide a comprehensive snapshot of the metabolites present in biological samples. This approach involves the identification and quantification of small molecules in biological samples such as blood, urine, or tissue. One of the key advantages of NMR-based metabolomics is its ability to analyze multiple metabolites simultaneously, to detect changes in metabolic pathways associated with various diseases. This can provide insights into disease mechanisms, identify potential biomarkers for early diagnosis, and monitor disease progression and response to treatment.NMR spectroscopy is a powerful tool for metabolomic analysis because it is non-destructive, requires minimal sample preparation, and can be used to analyze a wide range of metabolites, including sugars, amino acids, lipids, and organic acids. Furthermore, NMR spectra are highly reproducible, making it easier to compare results across different studies and laboratories.In human disease research, NMR-based metabolomics has been used to study a wide range of diseases, including cancer, diabetes, cardiovascular diseases, kidney disease, and neurological disorders. NMR spectroscopy has been used to identify metabolic signatures associated with diseases, which can help in early detection and personalized treatment strategies.Overall, NMR-based metabolomic approaches hold great promise for advancing our understanding of human diseases and improving diagnostic and therapeutic strategies.

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Symposium : **ANAL1-5**

Recent Status in NMR-based Analytical Chemistry

Room 103+104 THU 17:10

Chair: Youngbok Lee (Hanyang University)

Solid-state MAS NMR spectroscopic applications for polyanion cathode materials of Li-ion battery

Youngil Lee

Department of Chemistry, University of Ulsan, Korea

In the research and development of cathode materials for Li-ion battery, the analysis of the location and transfer channels of the Li-ion plays a crucial role. Solid-state NMR provides a great deal of information about the fine structure, the chemical structure, and the kinetics. Therefore, solid-state NMR analysis is widely used to develop cathode materials for Li-ion battery. Unlike solution NMR, solid-state NMR has a very wide spectral width. So, by using the MAS technique, which measures a magnetic resonance signal while rotating a solid powder sample at a specified angle at high speed, a high-resolution spectrum can be obtained to measure the local crystal structure change. In particular, solid-state MAS NMR has been widely utilized to investigate the local environment and electronic properties of Li, which is directly related to the operating efficiency of Li-ion battery. In this study, 7Li and 31P MAS NMR were used to analyze and compare the structural properties of polyanion materials (LixMy(XO4)z, M=Fe, Mn, Co, Ni; X=P, S, Si, B etc) as cathode materials for Li-ion battery. Information about the local electronic structure of the material was obtained for the spins and electrons of Li coupled within the paramagnetic material. Furthermore, by 7Li and 31P NMR shift, it was possible to analyze the crystal phase and the effect of phase change according to doping and coating of active materials to improve the electrochemical performance. Since these analyses are important for battery performance, MAS NMR studies of cathode materials will greatly contribute to the improvement of Li-ion battery performance and the development of new high-performance batteries.

Symposium : **ANAL2-1**

Recent Advances in Bioanalytical Chemistry

Room 103+104 FRI 14:30

Chair: Sungju Yu (Ajou University)

Analysis of Aggregated Protein Structure Changes in Brain Diseases Using Ion Mobility Mass Spectrometry (IM-MS)

Kun Cho

Division of Bioconvergence Analysis, Korea Basic Science Institute, Korea

The pathogenesis of brain disorders often involves the misfolding and aggregation of proteins, leading to neurodegeneration. Understanding the structural changes of these aggregated proteins is crucial for elucidating disease mechanisms and developing targeted therapies. Ion Mobility Mass Spectrometry (IM-MS) has emerged as a powerful tool for probing protein structures and dynamics at the molecular level. This research will delve into the principles and methodologies of IM-MS, highlighting its ability to discern complex protein conformations and transient intermediates. By applying IM-MS to study amyloid fibrils, oligomers, and other pathological protein aggregates implicated in neurodegenerative diseases, we seek to elucidate their structural dynamics and assembly pathways. Insights gained from IM-MS analyses offer valuable mechanistic insights into the assembly pathways of pathological protein aggregates and their interactions with cellular components. Additionally, we discuss the potential of IM-MS as a diagnostic tool for detecting disease-specific protein signatures in biological samples. By integrating IM-MS with complementary structural biology techniques, we envision a comprehensive approach to unraveling the complex architecture of protein misfolding diseases. Overall, the integration of IM-MS with other structural biology techniques holds great promise for advancing our understanding of protein misfolding diseases and facilitating the development of effective therapeutic interventions.

Symposium : **ANAL2-2**
Recent Advances in Bioanalytical Chemistry
Room 103+104 FRI 14:50
Chair: Sungju Yu (Ajou University)

Quantitative proteome analysis using data-independent acquisition in mass spectrometry for translational research

Kyunggon Kim

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

High resolution mass-spectrometry coupled with state-of-art protein/peptide separation technique have been applied on biology and translational area. And combination of other omics technology such as transcriptomics and genomics with proteomics have been extended the spectrum of its application to the precision medicine. This divergence phase of proteomics technology is playing an important and novel role as a name of proteo-genomics. At the same time, area of proteomics is reached to deep down of clinical unmet needs by not only instrument development but also deep understanding about the usefulness of proteomics application on translational research. Nowadays, proteomics also have been in convergence phase in clinical and translational area, especially in biomarker development and validation. In this presentation, most updated mass spectrometry methods, data-independent acquisition (DIA) approach to secure reproducibility and sensitivity of proteome will be introduced and its application for translational research will be presented.

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Symposium : **ANAL2-3**
Recent Advances in Bioanalytical Chemistry
Room 103+104 FRI 15:20
Chair: Seungah Lee (Kyung Hee University)

Monitoring Lipid Distribution and Gene Regulation of Lipid Expression in the Drosophila Head of Amyotrophic Lateral Sclerosis Model using Mass Spectrometry Imaging

Jin Gyeong Son

Nanobio Measurement Group, Korea Research Institute of Standards and Science, Korea

Lipid profile studies on complex nervous systems have mainly employed sample extraction and liquid chromatography-mass spectrometry (LC-MS) based analysis. However, this combined approach is a limited in obtaining spatiotemporal information of tissue samples. By combining time-of-flight secondary ion mass spectrometry (ToF-SIMS) and genetic techniques, we monitored lateral lipid changes in tissue of amyotrophic lateral sclerosis (ALS) models, one of the typical motor neurodegenerative diseases. To find out the molecular-level alteration in the early onset of ALS, we analyzed Drosophila early stages of head sections on days 1, 3, 5, and 9 after expression of G4C2 repeats. We discovered that the amounts of fatty acids, diacylglycerols, and ceramides increased in the fat body region of Drosophila heads at the early stage of disease progression (day 5), but before the onset of motor symptoms (day 10). To bring the upregulated lipids back to normal, we knocked down various genes involved in lipid metabolism to identify which related process changes. For this, we first identified several candidate genes that showed significant changes in the degree to which the ALS gene alleviated the eye pathology caused by the disease. Mass spectrometry image analysis confirmed that lipids were clearly downregulated in the FATP1 and ACBP genetic models, which showed the most significant eye recovery. This approach to studying ALS by monitoring gene regulation and lipid changes will help us understand the pathogenesis of other diseases.

Symposium : **ANAL2-4**

Recent Advances in Bioanalytical Chemistry

Room 103+104 FRI 15:40

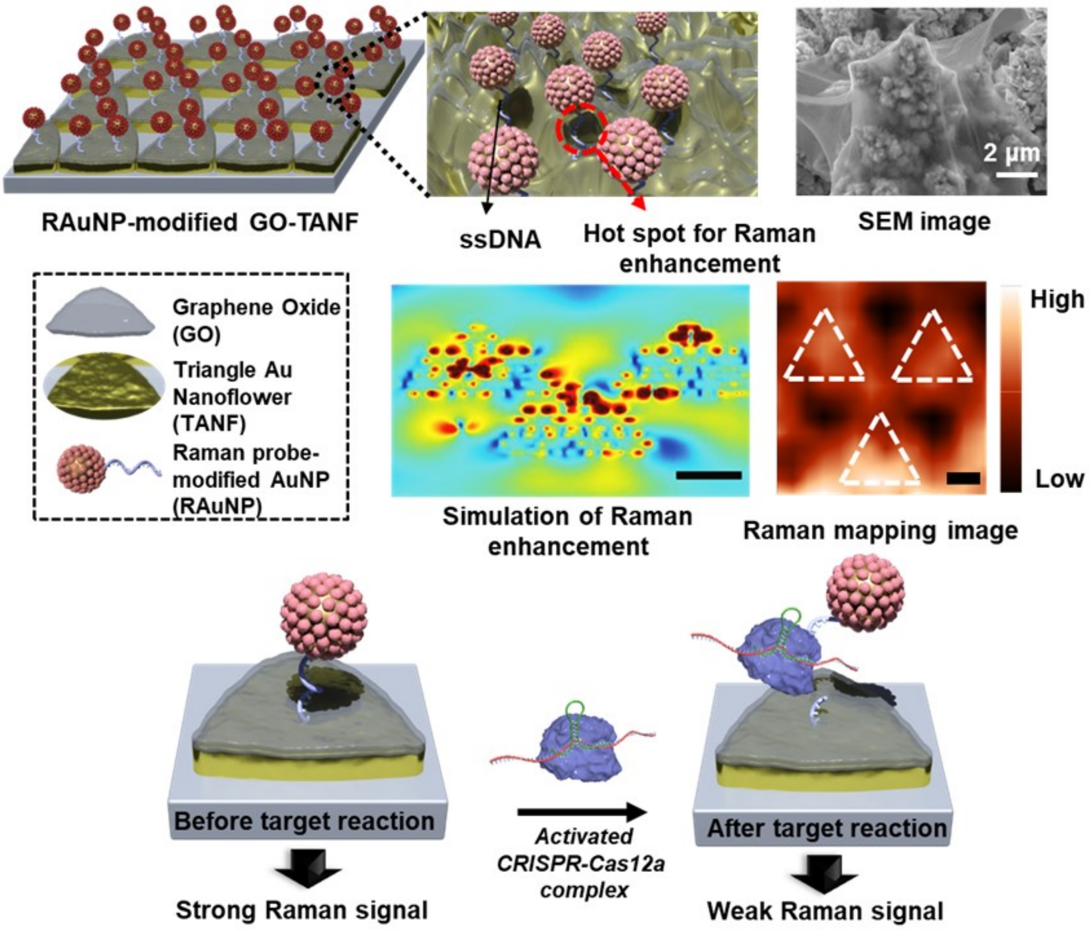
Chair: Seungah Lee (Kyung Hee University)

CRISPR-assisted plasmonic nanobiosensors for sensitive detection of disease-related biomarkers

Jin-Ha Choi

School of Chemical Engineering, Jeonbuk National University, Korea

CRISPR-based analytical strategies have gained attention for their simplicity and precision in diagnosing diseases, including SARS-CoV-2 and other highly contagious infectious diseases. However, sensitive detection typically requires crucial pre-amplification steps, such as polymerase chain reaction (PCR) or recombinase polymerase amplification (RPA), which are time-consuming and cost-ineffective. To overcome this limitation, we developed plasmonic nanomaterial-based highly sensitive nanobiosensors, including a metal-enhanced fluorescence (MEF)-assisted Au nanobiosensor and a surface-enhanced Raman spectroscopy (SERS)-based graphene oxide (GO)-Au nanoflower biosensor. Firstly, DNA-functionalized Au nanoparticles demonstrated excellent fluorescence enhancement by the activated CRISPR-Cas12a complex with target cell-free DNA (cfDNA, BRCA-1). On the other hand, the GO-Au nanoflower substrate enhanced Raman intensity and improved the sensitivity of multi-viral DNA detection, such as HBV, HPV-16, and HPV-18, without target amplification. We suggest that these CRISPR-Cas12a-based ultrasensitive and rapid detection systems can be widely applied for the precise and early diagnosis of fatal and highly infectious diseases.


RAuNP-modified GO-TANF
ssDNA
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2 µm
Graphene Oxide (GO)
Triangle Au Nanoflower (TANF)
Raman probe-modified AuNP (RAuNP)
High
Low
Simulation of Raman enhancement
Raman mapping image
Before target reaction
Strong Raman signal
Activated CRISPR-Cas12a complex
After target reaction
Weak Raman signal

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Symposium : **ANAL2-5**
Recent Advances in Bioanalytical Chemistry
Room 103+104 FRI 16:00
Chair: Seungah Lee (Kyung Hee University)

Chip-based fluorescent biosensing strategy measurement of model lipid membrane: ruptures and deformation.

Yong-Sang Ryu

School of Biomedical Engineering, Korea University, Korea

This presentation aims to elucidate the methodology of in-vitro cell membrane reconstitution and the real-time detection and observation of molecular-level physicochemical dynamics occurring on the cell membrane. In particular, various methods utilizing photophysical analysis will be described to track dynamic kinetic relationships of molecular chemistry. Furthermore, several examples will be presented to introduce the types of lipid components composing the cell membrane at the molecular level and their applications to disease diagnostic sensors.

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Symposium : **LIFE1-1**
Recent Advances in Disease-Targeted Drug Delivery System
Room 101+102 THU 15:40
Chair: Hak Joong Kim (Korea University)

Mechanistic Studies of the Radical SAM enzyme OxsB in Oxentanocin A Biosynthesis

Hung-wen Liu

University of Texas at Austin, United States

Radical S-adenosyl-L-methionine (SAM) enzymes are currently the largest known group of metalloenzymes and catalyze an extraordinarily broad range of chemical reactions via catalytic cycles involving free radical intermediates. All radical SAM enzymes are unified by the presence of an active site [Fe4S4] cluster that can reductively cleave SAM and thus initiate the radical-mediated catalytic cycle. A subgroup of radical SAM enzymes also bind cobalamin, which typically facilitates the methylation of substrate molecules at otherwise unactivated centers. However, OxsB is a cobalamin-dependent radical SAM enzyme that participates in the biosynthetic conversion of 2'-deoxyadenosine 5'-monophosphate (2'-dAMP) to the antiviral and antibiotic agent oxetanocin A, which contains a four-membered oxetane ring. Recent findings indicate that OxsB catalyzes an oxidative, intramolecular C–C bond formation in 2'-dAMP to yield a highly unstable intermediate. This intermediate undergoes facile nonenzymatic decomposition to produce an isomer of oxetanocin aldehyde phosphate. In the presence of the enzyme OxsA also from the oxetanocin A biosynthetic pathway, however, a regioselective bond cleavage is catalyzed to afford oxetanocin A aldehyde phosphate. Interestingly, OxsB can also catalyze radical mediated, stereoselective C2'-methylation of 2'-deoxyadenosine monophosphate. Moreover, subsequent rounds of catalysis result in C-C dehydrogenation of the newly added methyl group to yield a 2'-methylidene followed by radical addition of a 5'-deoxyadenosyl moiety to produce a heterodimer. These observations expand the scope of reactions catalyzed by B12-dependent radical SAM enzymes and emphasize the susceptibility of radical intermediates to bifurcation along different reaction pathways even within the highly organized active site of an enzyme.

133rd General Meeting of the Korean Chemical Society
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Symposium : **LIFE1-2**
Recent Advances in Disease-Targeted Drug Delivery System
Room 101+102 THU 16:10
Chair: Ja-Hyoung Ryu (UNIST)

Cancer-specific Prodrug Nanoparticles for Cancer Treatment

Kwangmeyung Kim

College of Pharmacy, Ewha Womans University, Korea

Prodrug nanoparticles are bio-reversible medication that undergo enzymatic or chemical transformation in vivo to release the active drug, which can exert desired pharmacological effect. This concept is now well established as a strategy to reduce severe toxicities of anticancer drugs by improving the cancer selectivity that can be activated in tumor microenvironment. Recently, many researchers more improved the pharmacokinetic (PK) characteristics of small-molecule prodrugs by nanoparticle-based drug delivery systems, which successfully enhanced the anticancer efficacy and reduced adverse effects. However, such approaches were mainly achieved by encapsulation or conjugation to polymeric-, lipid- or inorganic nanocarriers, thus showed low drug loading contents, in vivo toxicity by non-specific drug release and carrier itself. In addition, their unfavorable features for quality control (QC) and mass production hindered successful commercialization of prodrug nanomedicine. To overcome these limitations, our lab has focused on carrier-free cathepsin B-specific peptide-drug conjugates that from prodrug nanoparticles, and has published excellent results in many papers. Herein, we want to introduce these researches with recent advances and progress for prodrug nanoparticles for cancer treatment.

Symposium : **LIFE1-3**
Recent Advances in Disease-Targeted Drug Delivery System
Room 101+102 THU 16:35
Chair: Ja-Hyoung Ryu (UNIST)

Multiscale and Hierarchical Assembly for Advanced Photomedicine

Sehoon Kim

Korea Institute of Science and Technology, Korea

Light-guided and/or light-activated phototherapy is a noninvasive and selective treatment modality for cancer and other diseases. The therapeutic effect is triggered by colocalization of photomedicine and light irradiation at the site of action (diseased target tissue), through which the photon energy absorbed by PS is transferred to the environment to generate reactive oxygen species (ROS) to kill disease cells directly (via photodynamic therapy) or sensitize the environment to the subsequent therapeutic intervention. Supramolecular and/or organic-inorganic assemblies often potentiate proper delivery of photomedicine to the target tissues/cells, as well as another intriguing effect on the photophysical properties that govern the efficiency of photosensitizaton; i.e., smart control of the molecular interaction in the assembly can switch the phototherapeutic activity on demand, enabling safer and more precise phototherapy.In this presentation, our recent results on multiscale and hierarchically assembled photomedicine approaches at molecular-micro-bulk levels will be introduced, including (1) a photosensitizer/quencher-linked peptide monolith that can assemble into further photosensitization-quenched bulk depot upon tissue injection, (2) photoechogenic inflatable nanohybrids where an upconversion nanoparticle core converts low-energy NIR photons into high-energy ultraviolet emission for hierarchical photolysis of the gas generator, gas generation carbon and inflation into microbubbles for light-guided sonotheranostics, and (3) heavy-atom enhanced nanophotosensitizer for photoimmunotherapy.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **LIFE1-4**

Recent Advances in Disease-Targeted Drug Delivery System

Room 101+102 THU 17:00

Chair: Youngdo Jeong (KIST)

Glycocalyx-mimicking nanoparticles for cell and tissue-selective drug delivery

Sangyong Jon

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

The glycocalyx is a pericellular carbohydrate coat that is ubiquitously present on cells and crucially contributes to numerous biological processes, such as cell-cell recognition, cell-extracellular matrix interactions, cell adhesion, etc. The heterogenous sugar moieties of a cell’s glycocalyx can be multivalently recognized by another cell’s receptors, lectins, and/or glycocalyx. We speculated that the types, compositions, and spatial arrangement of individual sugar moieties of a glycocalyx may determine its binding affinity and selectivity for target cells. We thus hypothesized that a library of glycocalyx-mimicking nanoparticles (designated GlyNPs) could be used to screen and identify GlyNP hits with desired tissue or cell tropisms. We very recently published papers in which we used GlyNP libraries to identify cancer type-selective nanoparticles for tumor imaging and therapy (Adv. Mater. 2022: 34, 2203993) and a nanomedicine capable of targeting and treating inflamed colon through direct in vivo screening of a mouse colitis model (Angew. Chem. Int. Ed. 2023: 62, e202304815). In this talk, I will present a GlyNP library that can be leveraged for direct in vivo screening and identification of organ-selective nanoparticles and furthermore, the use of the organ-selective GlyNPs for treatments of organ-associated diseases.

Symposium : **LIFE1-5**

Recent Advances in Disease-Targeted Drug Delivery System

Room 101+102 THU 17:25

Chair: Youngdo Jeong (KIST)

pH-responsive peptides for selective drug delivery

Yan Lee

Division of Chemistry, Seoul National University, Korea

In this presentation, two examples of drug delivery vehicles based on pH-responsive peptides, which are designed for targeting infected tissues or cancerous tissues, are introduced. In the first part, peptide sequences with pH-selective membrane-perturbing activity are introduced. These peptides permeabilize the outer membrane of gram-negative bacteria without demolishing it, and specifically increase the influx of nonpermeable antibiotics only under acidic pH. Moreover, metabolic stability studies show that these peptides were more stable than peptides with permanent positive charges primarily due to reduced recognition by the mononuclear phagocyte system. These peptides demonstrate high therapeutic efficacy in a multi-drug resistant A. baumannii infection model, while showing reduced host toxicity.In the second part, a pH-responsive linker based on natural amino acids for selective delivery of protein pharmaceuticals is introduced. A self-cleaving protein, pH inteinN150, can be obtained by mutation of key amino acids in the original pH intein. By using the pH inteinN150 linker, the intracellular penetration of protein cargos can be selectively turned on or off at weakly acidic pH. Furthermore, a recombinant protein in which human necrosis factor-related death-inducing ligand (hTRAIL) was fused with albumin binding domain (ABD) via the pH inteinN150 linker can be obtained. The apoptosis-inducing activity of hTRAIL can be selectively activated by cleaving the linker at weakly acidic pH in tumors of a xenograft mouse model. We expect that these new pH-responsive peptide sequences can be used for actively controlling various pharmaceuticals responding to delicate pH variations around inflammatory or cancerous tissues.

Symposium : **LIFE2-1**
Recent Trends in Structural Biochemical Research
Room 101+102 FRI 09:00
Chair: Hyun Kyu Song (Korea University)

Polymorphic self assembly of DegQ protein inspired by Origami strategies

Ingyun Lee

College of Pharmacy, Seoul National University , Korea

As large molecular tertiary structures, some proteins can act as small robots that find, bind, and chaperone target protein clients, showing the potential to serve as smart building blocks in self-assembly fields. Instead of using such intrinsic functions, most self-assembly methodologies for proteins aim for de novo-designed structures with accurate geometric assemblies, which could limit procedural flexibility. Here, we present a strategy enabling polymorphic clustering of quaternary proteins, exhibiting simplicity and flexibility of self-assembling paths for proteins in forming monodisperse quaternary cage particles. We propose that the enzyme protomer DegQ, previously solved at low resolution, may potentially be usable as a threefold symmetric building block, which can form polyhedral cages incorporated by the chaperone action of DegQ in the presence of protein clients. To obtain highly monodisperse cage particles, we utilize soft, and hence, less resistive client proteins, which can program the inherent chaperone activity of DegQ to efficient formations of polymorphic cages, depending on the size of clients. By reconstructing the atomic resolution cryo-EM DegQ structures using obtained 12- and 24-meric clusters, we validate the polymorphic clustering of DegQ enzymes in terms of soft and rigid domains, which would provide effective routes for protein self-assemblies with procedural flexibility.

Symposium : **LIFE2-2**
Recent Trends in Structural Biochemical Research
Room 101+102 FRI 09:30
Chair: Hyun Kyu Song (Korea University)

Metal Binding Proteins with Metal Selectivity or Enzymatic Activity

Tae Su Choi

Division of Life Sciences, Korea University, Korea

Metalloproteins play crucial roles in living organisms, managing metal homeostasis and catalyzing enzymatic reactions Central to the functions of metalloproteins is metal coordination, where each metalloprotein must pair with the appropriate metal cofactor to carry out its biological tasks. In this presentation, I will discuss methods for designing artificial metalloproteins using flexible protein scaffolds mediated by disulfide bonds, and explore the biochemical insights gleaned from these designed proteins.The inherent flexibility of protein structures can interfere with the specific selection of metal ions, whose electron configurations dictate preferred coordination geometries. Consequently, many metalloproteins tend to conform to the Irving-Williams (IW) series series (Mn(II) < Fe(II) < Co(II) < Ni(II) < Cu(II) > Zn(II)) in terms of metal-protein binding affinities. This trend leads to the loss of intrinsic structural or catalytic functions of metalloproteins. I will delve into the design and characterization of artificial dimeric proteins engineered to overcome these IW restrictions both in vitro and in cellulo. These proteins favor the binding of lower-IW transition metals over Cu(II), which is the most dominant ion in the IW series.The flexible dimer scaffold can be systematically adapted to create metalloprotein variants with enzymatic activity. By positioning metal binding residues variably within the flexible interface, diverse metal coordination spheres are formed, resulting in an entatic state of the metal ion with superoxide dismutase-like activity. I will outline a simulation strategy for predicting potential combinations of metal coordination sites within the flexible dimer interface, as well as the experimental validation of enzymatic activity stemming from these predictions.

Symposium : **LIFE2-3**
Recent Trends in Structural Biochemical Research
Room 101+102 FRI 10:00
Chair: Hyun Kyu Song (Korea University)

Structural Basis for Rab1 Glucosylation by Legionella SetA on the Early Legionella-Containing Vacuole

Hyoun Sook Kim

Targeted Therapy Branch, National Cancer Center, Korea

Legionnaires' disease, a severe form of pneumonia primarily targeting the elderly and immunocompromised, is on the rise in the industrialized world due to Legionella pneumophila. This bacterium has honed its virulence through long-term coevolution with aquatic protozoa, enabling it to infect a wide range of phagocytic eukaryotes, including humans. Central to its pathogenicity is the establishment of the Legionella-containing vacuole (LCV) within host cells, facilitated by the Dot/Icm type IV secretion system, which delivers a suite of effector proteins to manipulate host cellular processes. Among these, Legionella glucosyltransferases, specifically SetA, have emerged as pivotal in altering host cell functions through the modification of key signaling molecules like Rab1 via glycosylation. This study delves into the structural and molecular underpinnings of Rab1 glycosylation by SetA, examining the enzyme's interaction with various ligands, including phosphatidylinositol-3-phosphate (PI3P), crucial for early LCV formation. Through a combination of crystallography, biochemical assays, biophysical techniques, in silico docking, and SAXS studies, we provide a comprehensive view of SetA's action mechanism, highlighting its specificity for GDP-bound Rab1 and PI3P. These insights shed light on Legionella's intricate evasion of host immune responses, offering a foundation for future therapeutic strategies against Legionnaires' disease.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **LIFE2-4**

Recent Trends in Structural Biochemical Research

Room 101+102 FRI 10:30

Chair: Hyun Kyu Song (Korea University)

Understanding the structural basis of Mutipass membrane protein biogenesis

Minkyung Kim

College of Pharmacy, Gachon University, Korea

Multipass membrane proteins play a crucial role in physiological processes. However, the mechanisms of correct insertion and folding into the cell membrane remain unclear. Prevailing models suggest that multipass membrane proteins are inserted iteratively through a lateral gate in the Sec61 protein translocation channel in the ER. The PAT complex, an intramembrane chaperone comprising Asterix and CCDC47, contacts early TMDs of multipass proteins to promote their biogenesis via an unknown mechanism. Here, structural and biochemical analysis of intermediates during multipass protein biogenesis discovered that the nascent chain is not engaged with Sec61 but is instead obstructed and secured closed by CCDC47. Asterix binds to the substrate, redirecting it to a position behind Sec61, where the PAT complex contributes to a multipass translocon surrounding a partially enclosed, lipid-filled cavity. Detection of multiple TMDs in this cavity after their emergence from the ribosome suggests that multipass proteins insert and fold behind Sec61. Thus, the biogenesis of several multipass proteins was unimpeded by inhibitors of the Sec61 lateral gate. These findings provide insights into the mechanism of an intramembrane chaperone and propose a new framework for understanding multipass membrane protein biogenesis in the endoplasmic reticulum.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

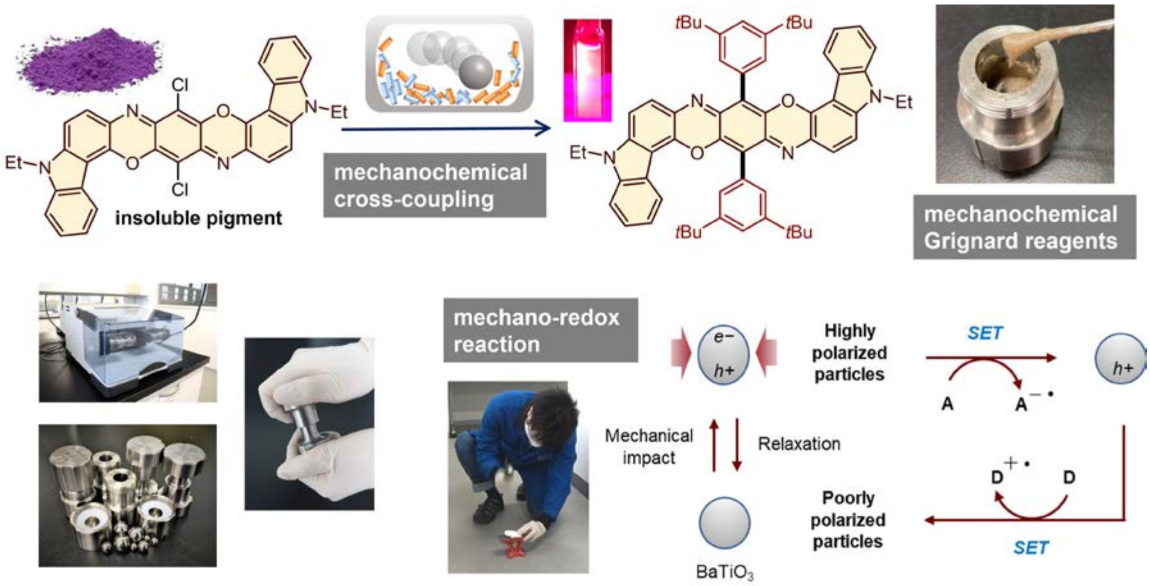
Symposium : **ORGN1-1**
Leading Research Symposium on Organic Chemistry
Room 304+305+306 THU 09:15
Chair: Jeung Gon Kim (Jeonbuk National University)

Mechanochemistry for efficient organic synthesis: Our latest study

Hajime Ito

Hokkaido University, Japan

Mechanochemical synthesis uses little or no solvent. It is an alternative to conventional organic synthesis in solution. Instead of using a solvent and standard glassware, mechanochemical reactions are carried out with the aid of a ball mill or other grinding device. In addition to the reduced use of organic solvents, this method offers several advantages, such as accelerated reactions due to high concentration conditions, the ability to react with insoluble compounds, the activation of substrates by physical forces, and increased selectivity in a solid phase. Exploiting these advantages, we have reported Suzuki coupling of insoluble compounds, performed "mechanoredox" reactions using piezoelectric materials, synthesized organometallic compounds such as "Grignard reagents by ball milling", and achieved "ultra-fast one minute Birch reduction". This talk will present our latest research on the potential of this technique and its impact on the field of organic synthesis.


Cl
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O
N-Et
Et-N
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Cl
insoluble pigment
mechanochemical cross-coupling
tBu
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O
N
tBu
tBu
mechanochemical Grignard reagents
mechano-redox reaction
e−
h+
Highly polarized particles
SET
A
A−•
h+
Mechanical impact
Relaxation
D+•
D
BaTiO3
Poorly polarized particles
SET

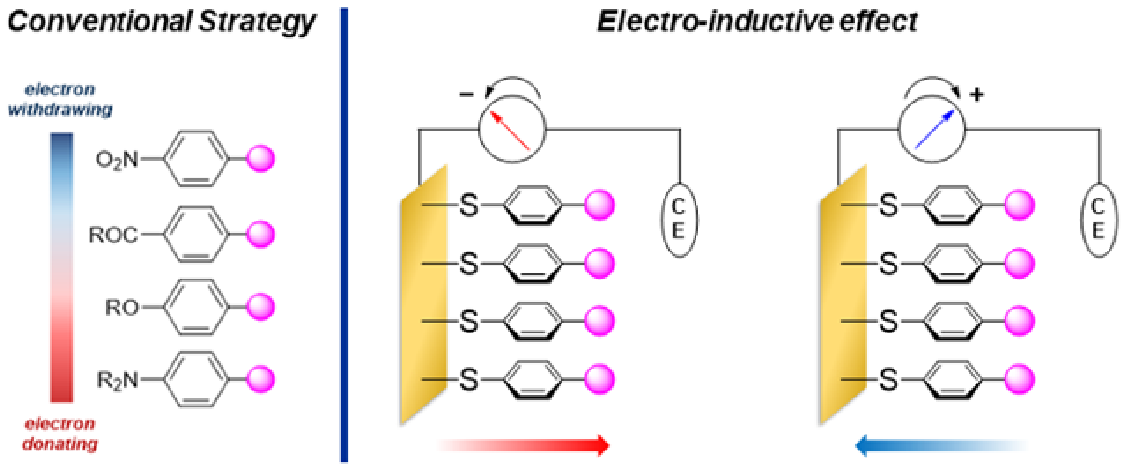
Symposium : **ORGN1-2**
Leading Research Symposium on Organic Chemistry
Room 304+305+306 THU 09:50
Chair: Jeung Gon Kim (Jeonbuk National University)

Progress towards using the electro-inductive effect to control organic reactions.

Mu-Hyun Baik

Chemistry, Korea Advanced Institute of Science and Technology, Korea

In 2020, we reported that electrodes can be used as a universal functional group with adjustable inductive effect (Science 2020, 370, 214-219): Placing a reactive molecule on the surface of an electrode, we can apply negative voltage to push electron density into the molecule, mimicking the effect of decorating the molecule with electron-donating functional groups. Positive voltage has the effect of adding electron-withdrawing groups. In this presentation, I will offer an update on our efforts to go beyond the proof-of-principle studies and move towards controlling the outcome of organic reactions at a larger scale. Employing carbon electrodes, we were able to change the yield and stereoselectivity of simple organic reactions at NMR-detectable scales.


Conventional Strategy
electron withdrawing
O_2N
ROC
RO
R_2N
electron donating
Electro-inductive effect
–
+
S
C E

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

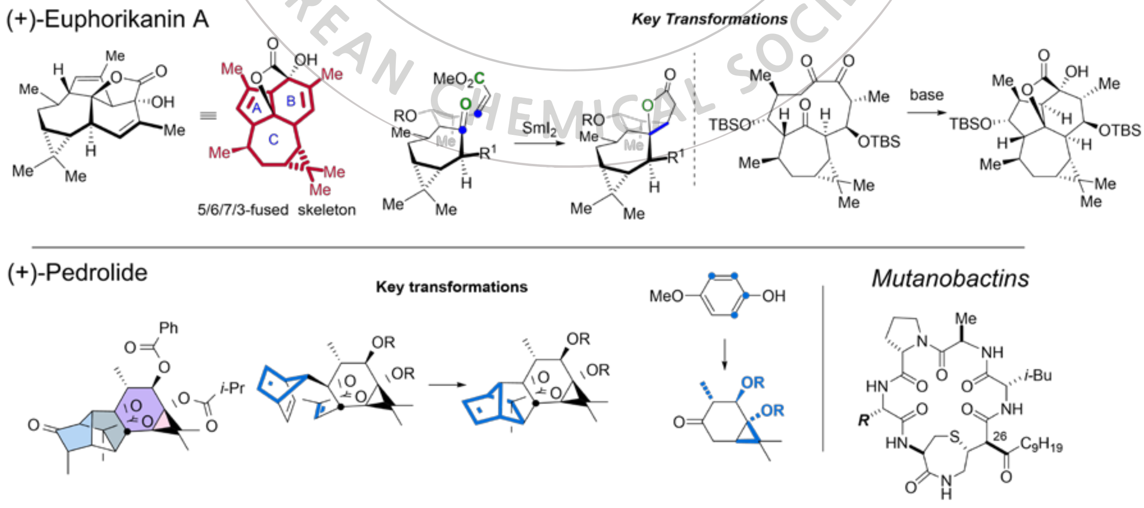
Symposium : **ORGN1-3**
Leading Research Symposium on Organic Chemistry
Room 304+305+306 THU 10:25
Chair: Jeung Gon Kim (Jeonbuk National University)

New Strategies and Tactics in Natural Products Synthesis

Erick M. Carreira

ETH-Zürich, Zürich, Switzerland, Switzerland

The presentation will include discussion and analysis of recent natural product targets that have been synthesized in the group. It will focus on target-oriented synthesis as an engine for the generation of novel methods and approaches to bioactive agents. The methods involve novel, unexpected reactivity and unusual building blocks that are fully integrated to lead to efficient routes. We will focus specifically on recently completed syntheses.



133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **ORGN2-1**
Current Trends in Organic Chemistry
Room 304+305+306 FRI 09:00
Chair: Jung Min Joo (Kyung Hee University)

Catalytic Control of Atropisomerism through Dynamic Kinetic Resolution

Yongseok Kwon

School of Pharmacy, Sungkyunkwan University, Korea

The significance of atropisomerism has been emphasized in the field of asymmetric catalysis, leading to the development of numerous recent reactions. Various synthetic methods for the selective synthesis of atropisomers can be categorized into several strategies, among which dynamic kinetic resolution stands out as an attractive approach by harnessing the rotational flexibility of substrates. In this regard, we report the development of an atroposelective Pictet-Spengler cyclization employing dynamic kinetic resolution. This reaction was applicable to two distinct substrate types, allowing for the control of axial chirality in both C−N and C−C single bonds. By introducing functional groups capable of forming hydrogen bonds on the opposite aromatic ring, remarkably high enantioselectivity was achieved. Furthermore, the reaction was extended to intermolecular reactions, demonstrating a method to control atropisomerism by introducing an activated ketone into indole. It was shown that control over positions N-1, C-2, and C-3 of indole could be achieved. Furthermore, computational investigations have been conducted to provide deeper insights into the origin of enantioselectivity.

Symposium : **ORGN2-2**

Current Trends in Organic Chemistry

Room 304+305+306 FRI 09:30

Chair: Jung Min Joo (Kyung Hee University)

Ortho-heteroatom-substituted aryl phosphorus compounds by three-component coupling reactions

Seojung Han

Chemical and Biological Integrative Research Center, Korea Institute of Science and Technology, Korea

Arynes play a crucial role as synthetic intermediates, facilitating the 1,2-difuntionalization of aromatic rings. This distinct class of chemical compound is extensively employed in the synthesis of functional polycyclic aromatic rings, architecturally complicated bioactive molecules, and natural products. In this presentation, we describe an efficient, mild, metal-free and straightforward method for the synthesis of *ortho*-silicon substituted aryl phosphonate by three-component coupling reactions involving arynes, phosphites, and silyl fluorides. An array of *ortho*-silicon substituted aryl phosphonates can be produced using various silyl fluorides with a broad functional group tolerance in moderate to good yields. In the second part of this presentation, we describe a synthetic strategy toward *ortho*-halogen substituted aryl(alkynyl)phosphinates by three-component coupling reaction involving arynes, phosphites, and haloalkynes. This mild and metal-free method allows direct access to various *ortho*-halogen substituted aryl(alkynyl)phosphinates in moderate to good yields in a single step. This reaction can be utilized for synthesizing diverse organophosphorus compounds present in natural products, materials, and bioactive molecules.

Symposium : **ORGN2-3**
Current Trends in Organic Chemistry
Room 304+305+306 FRI 10:00
Chair: Jung Min Joo (Kyung Hee University)

Copper-Mediated Preparation of N-Aryl Amides from Dioxazolones with Arylboronic Acids

Jongwoo Son

Department of Chemistry, Dong-A University, Korea

Dioxazolones, potent amide precursors, have been investigated for the N-arylation with the help of transition-metal catalysts. Here, we present our recent studies on the synthesis of N-aryl amides using dioxazolones and boronic acids in the presence of copper(I) chloride under mild conditions. The synthetic utility is represented by its wide range of dioxazolones. The reaction optimization screenings indicated that a fluorine additive exhibited improved reactivity toward the desired transformation. The addition of organophosphines results in N-acyl iminophosphoranes, suggesting the involvement of an N-acyl nitrene intermediate in this transformation.

133rd General Meeting of the Korean Chemical Society
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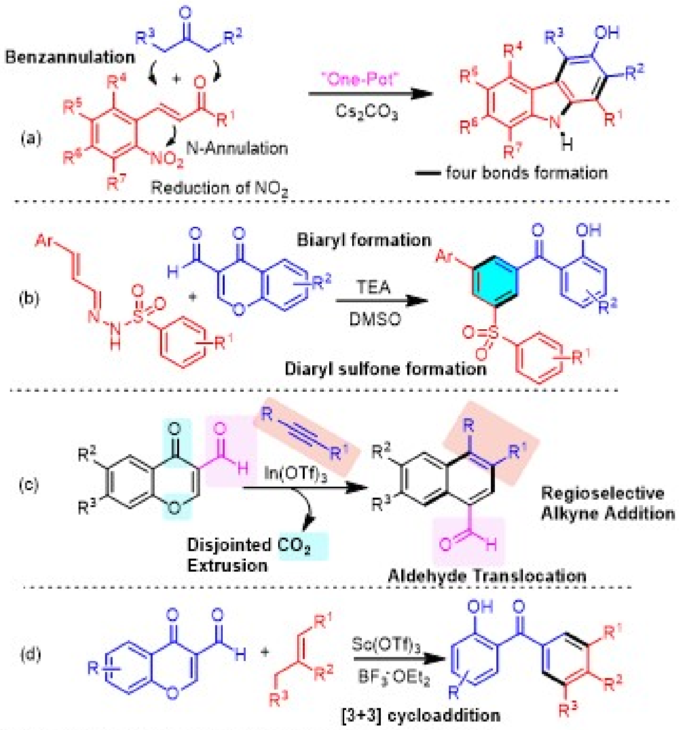
Symposium : **ORGN2-4**
Current Trends in Organic Chemistry
Room 304+305+306 FRI 10:30
Chair: Jung Min Joo (Kyung Hee University)

Construction of Biologically Interesting Aromatics via Benzannulation

Yong Rok Lee

School of Chemical Engineering, Yeungnam University, Korea

The benzannulation reaction has been widely used in the synthesis of diversely functionalized aromatic molecules with myriad properties. The construction of functionalized and diverse aromatic via benzannulation plays a vital role in advanced synthetic organic chemistry. Recently, we have interested in the synthesis of aromatics and heteroaromatics via benzannulation. In this presentation, we describe facile and efficient synthetic approaches of biologically interesting aromatics such as carbazoles, biaryls, xanthones, biarylsulfones, naphthaldehydes, and 2-hydroxybenzophenones via benzannulation (Scheme 1).



Scheme 1. Synthetic strategies for aromatics via benzannulation

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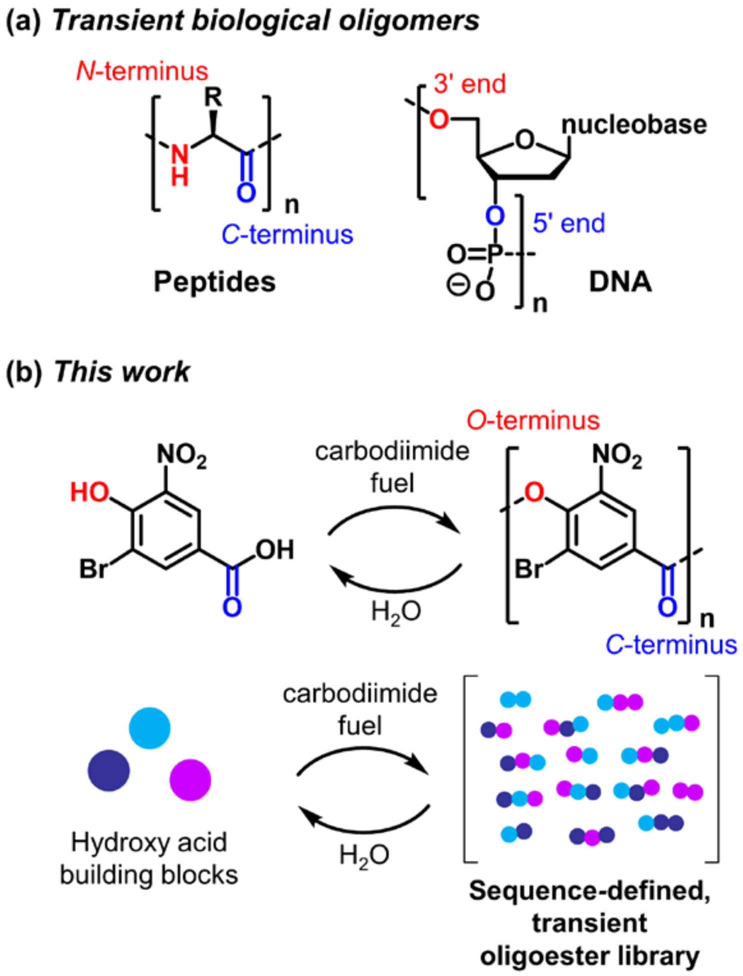
Symposium : **ORGN3-1**
Current Trends in Chemosensors
Room 304+305+306 FRI 14:30
Chair: Min Hee Lee (Chung-Ang University)

Chemically fueled dissipative oligoester library

Sunbum Kwon

Department of Chemistry, Chung-Ang University, Korea

A key characteristic of major biopolymers like nucleic acids and proteins is their constant turnover within living cells. Biopolymers are synthesized from their monomeric units with the aid of energy sources, but they also undergo spontaneous degradation back into monomers in aqueous environments. Inspired by these dynamic systems observed in nature, significant research has focused on creating artificial systems that operate out-of-equilibrium under controlled conditions. However, creating systems that involve transient oligomers with specific directional properties has proven challenging. In this study, we conduct a comprehensive kinetic analysis of the chemical reaction network involved in the carbodiimide-fueled dissipative oligomerization of hydroxybenzoic acids. This process is accompanied by functional diversification based on the sequence of building blocks. We anticipate that the discovery of new transient oligomers with directional properties, along with their associated chemical fuels, may provide a unique opportunity to design innovative out-of-equilibrium systems capable of mimicking complex biological processes.


(a) Transient biological oligomers
N-terminus
R
N
H
O
n
C-terminus
Peptides
3' end
O
O
nucleobase
O
5' end
O=P
⊖O
n
DNA
(b) This work
NO2
HO
Br
OH
O
carbodiimide fuel
H2O
O-terminus
NO2
O
Br
O
n
C-terminus
Hydroxy acid building blocks
carbodiimide fuel
H2O
Sequence-defined, transient oligoester library

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **ORGN3-2**
Current Trends in Chemosensors
Room 304+305+306 FRI 14:55
Chair: Min Hee Lee (Chung-Ang University)

Macrocyclic ion pair receptors for the extraction of lithium salts

Sung Kuk Kim

Department of Chemistry, Gyeongsang National University, Korea

The development of an effective method for selective extraction of lithium salts from lithium sources such as rocky ores and salt-lake brine has attracted increasing attention as the demand for lithium is explosively increasing. This presentation will be focused on our efforts to develop extractants capable of selectively extracting a lithium salt in the solid state and from an aqueous solution. To this end, we constructed various ion pair receptors by combining various lithium-selective cation binding motifs with macrocyclic pyrrolic anion binding sites. In contrast to simple ion receptors which bind either an anion or a cation, an ion pair receptor often binds both an anion and a cation concurrently with enhanced affinity and selectivity. Effects of solvents and spectator ions on lithium extraction by the ion pair receptors will be also discussed. As time permits, a calix[4]pyrrole dimer whose ability to bind the fluoride anions with 1:2 stoichiometry is remarkably promoted by the dihydrogen phosphate anion will be also presented.

133rd General Meeting of the Korean Chemical Society
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Symposium : **ORGN3-3**
Current Trends in Chemosensors
Room 304+305+306 FRI 15:20
Chair: Min Hee Lee (Chung-Ang University)

Indolizine-based fluorescent compound arrays for machine learning-assisted chemical sensing

Eunha Kim

Department of Molecular Science and Technology, Ajou University, Korea

Among various sensing systems, fluorometric sensors have been widely used in various chemical sensing applications because of their high sensitivity and broad applicability in different settings. The fundamental understanding of fluorophores photophysical properties related to their structures and the advances of supramolecular chemistry synergistically have led to the discovery of various sensitive fluorescent sensors. Despite enthusiastic endeavors, however, it remains challenging to develop cost-effective, high-precision, and broadband working paper-type fluorescent sensing systems, particularly for on-site or in-the-field sensing applications. Recently, we developed paper-based Point-of-Care (POC) sensing arrays consisting of indolizine-based fluorescent compounds. Using an indolizine structure as a fluorescent core skeleton, several libraries were designed and synthesized. We found the fluorescent chemical arrays could be useful for discrminating Volatile Organic Compounds, measuring pH of the aqueous solution, and determining concentration of glucose in biological sample. In addition, more importantly, we also demonstrate that the paper-based POC testing systems powered by machine learning could providing significantly improved accuracy and robustness.

Symposium : **ORGN3-4**
Current Trends in Chemosensors
Room 304+305+306 FRI 15:45
Chair: Min Hee Lee (Chung-Ang University)

Dis/aggregation dependent fluorescent chemosensors for bioimaging applications

Jun-Seok Lee

Department of Pharmacology, Korea University, Korea

Fluorescent organic dyes hold significant promise for diverse applications, particularly in the realm of biological imaging. Within this domain, two distinct categories of fluorescence agents have emerged: bright fluorophores serving as imaging tags for endogenous biomolecules and fluorescent molecules capable of dynamic responses as biosensors. Our research group is dedicated to advancing these fields through the development of novel chemosensors and investigating their mechanisms of action. In recent investigations, our research team has undertaken an extensive exploration of fluorescence-based chemosensors, focusing particularly on the development and characterization of chemosensors reliant on the aggregation state. Through meticulous synthesis endeavors, we have successfully curated a 48-membered combinatorial fluorescent library anchored on the dansyl scaffold. This library has undergone rigorous bioanalyte screening and structural analysis, revealing intriguing selectivity towards progesterone with a turn-on effect and demonstrating substantial potential for applications in aggregation-dependent biosensing. Leveraging this foundational work, we are now extending our methodology to include the deliberate design and synthesis of BODIPY-based drug conjugates tailored for precise fixed tissue imaging purposes. This comprehensive strategy not only underscores our steadfast dedication to advancing fluorescence-based chemosensing but also aims to address specific imaging requisites across various biological contexts. Through meticulous characterization and rigorous evaluation, our objective is to unearth novel insights and forge pathways for innovative applications within the realms of analytical and biological sciences.

Symposium : **MEDI1-1**
The Cutting Edge of Medicinal Chemistry
Room 301+302 THU 15:40
Chair: Ji Hoon Lee (KMEDIhub)

Novel TPD Selectively Targeting KRAS-G12D Mutant

Taebo Sim[*]**, Eunhye Jeon, Chan Kim**

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

KRASG12D is the most prevalent KRAS mutant in various cancers. We have recently identified a selective KRASG12D protein degrader capable of degrading selectively KRASG12D over other KRAS mutants as well as KRASWT. A series of PROTACs were rationally designed, synthesized, and evaluated on HeLa cells expressing eGFP-fused KRASG12D protein and AsPC-1 cells, which led to identification of a lead, YUH91138. The binding site of YUH91138 on KRASG12D was identified by 1H-15N HSQC NMR studies and ternary complex formation was determined by nanoBRET assay. In addition, YUH91138 suppresses proliferation of AsPC-1 cells via KRAS signaling blockade, apoptosis and blocks migration and invasion of AsPC-1 cells. Moreover, YUH91138 inhibits colon cancer patient-derived organoids (PDO) harboring KRASG12D but no PDO with KRASWT. Furthermore, YUH91138 possesses significant efficacies in AsPC-1 tumor xenograft mouse model.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **MEDI1-2**
The Cutting Edge of Medicinal Chemistry
Room 301+302 THU 16:10
Chair: Ji Hoon Lee (KMEDIhub)

Discovery of novel anti-cancer candidate targeting Pin1 isomerase

Sang Hyun Min

Department of Innovative New Drug, Kyungpook National University, Korea

Protein phosphorylation and post-phosphorylation events regulate many cellular signaling pathways. Peptidyl-prolyl isomerase (Pin1) is the only peptidyl-prolyl cis/trans isomerase (PPIase) that interacts with numerous oncogenic or tumor suppressive phosphorylated proteins, causes conformational changes in target proteins, and eventually regulates the activities of such proteins. These alterations in activity play a pivotal role in tumorigenesis. Since Pin1 is overexpressed and/or activated in various types of cancers especially in breast cancer, and the dysregulation of proline-directed phosphorylation contributes to tumorigenesis, Pin1 represents an attractive target for breast cancer therapy. I will describe the role of Pin1 in cancer and the current status of Pin1 inhibitor development. Keywords: Proline-directed phosphorylation, cancer-driving pathways, tumorigenesis, Pin1, Pin1 inhibitor, Prolyl isomerase

Symposium : **MEDI1-3**

The Cutting Edge of Medicinal Chemistry

Room 301+302 THU 16:40

Chair: Ji Hoon Lee (KMEDIhub)

Novel Recombinant Human Hyaluronidase

Kyuwan Kim

New Drug Development, Alteogen, Korea

Hyaluronidase is an enzyme that hydrolyzes hyaluronic acid and has been used in the fields of cancer treatment, wound healing, ophthalmological application, cosmetological application, and infertility treatment, and is also used for subcutaneous delivery of medicines. When administering an injection into the dense subcutaneous tissue composed of collagens and hyaluronic acids, the use of the hyaluronidase reduces the density of the subcutaneous tissue and can be developed as an administration route for various medicines. In the case of poorly soluble medicines that require large-dose and repetitive administration, anesthetics that require rapid efficacy, or high-molecular-weight medicines like antibody drugs, hyaluronidases can be administered subcutaneously through parallel or mixed administration with medicines, increasing treatment convenience and effectiveness of medicines. Hyaluronidase products have been commercialized using substances purified from animal testicles, but with the launch of recombinant hyaluronidase manufactured from sequences that exist in nature, the therapeutic field has expanded to broad spectrum of medicines.Alteogen developed a novel recombinant hyaluronidase, ALT-B4, which has superior immunogenicity, heat stability, and enzymatic activity compared to the existing recombinant hyaluronidase, using protein design technology that combines two types of human hyaluronidase. The ALT-B4 project is expanding the therapeutic area through collaboration with companies with various APIs, and based on excellent productivity, it is entering the hyaluronidase market with a product called Tergase by 2024.

Symposium : **MEDI1-4**

The Cutting Edge of Medicinal Chemistry

Room 301+302 THU 17:10

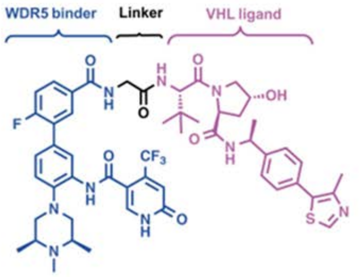
Chair: Ji Hoon Lee (KMEDIhub)

Discovery of PROTACs; Turning undruggable targets into druggable targets

Kwang-Su Park

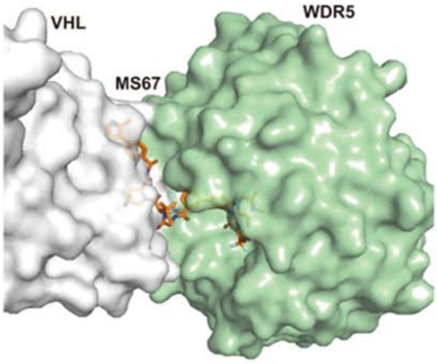
College of Pharmacy, Keimyung University, Korea

PROteolysis TArgeting Chimeras (PROTACs) represent an evolving therapeutic paradigm that exhibits promise in addressing disease-associated proteins traditionally resistant to conventional small-molecule targeting. Since the inception of the PROTAC concept two decades ago, leveraging the ubiquitin–proteasome system for targeted protein degradation, PROTAC has transitioned from academic exploration to substantial industry involvement. Multiple companies have introduced preclinical and early clinical development programs, signifying a notable shift towards real-world applications. This technology holds potential advantages over traditional inhibitors, particularly in mitigating off-target effects, overcoming drug resistance, and targeting previously deemed undruggable proteins. Today, I'd like to provide a comprehensive summary of the initial two decades of PROTAC discovery, offering insights into the current landscape with a specific focus on the academic perspective.



MS67

Chemical Structure of WDR5 targeting PROTAC (MS67)



Crystal Structure of PROTAC (MS67) with Target Protein (WDR5) and E3 ligase (VHL) (PDB ID: 7JTP)

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

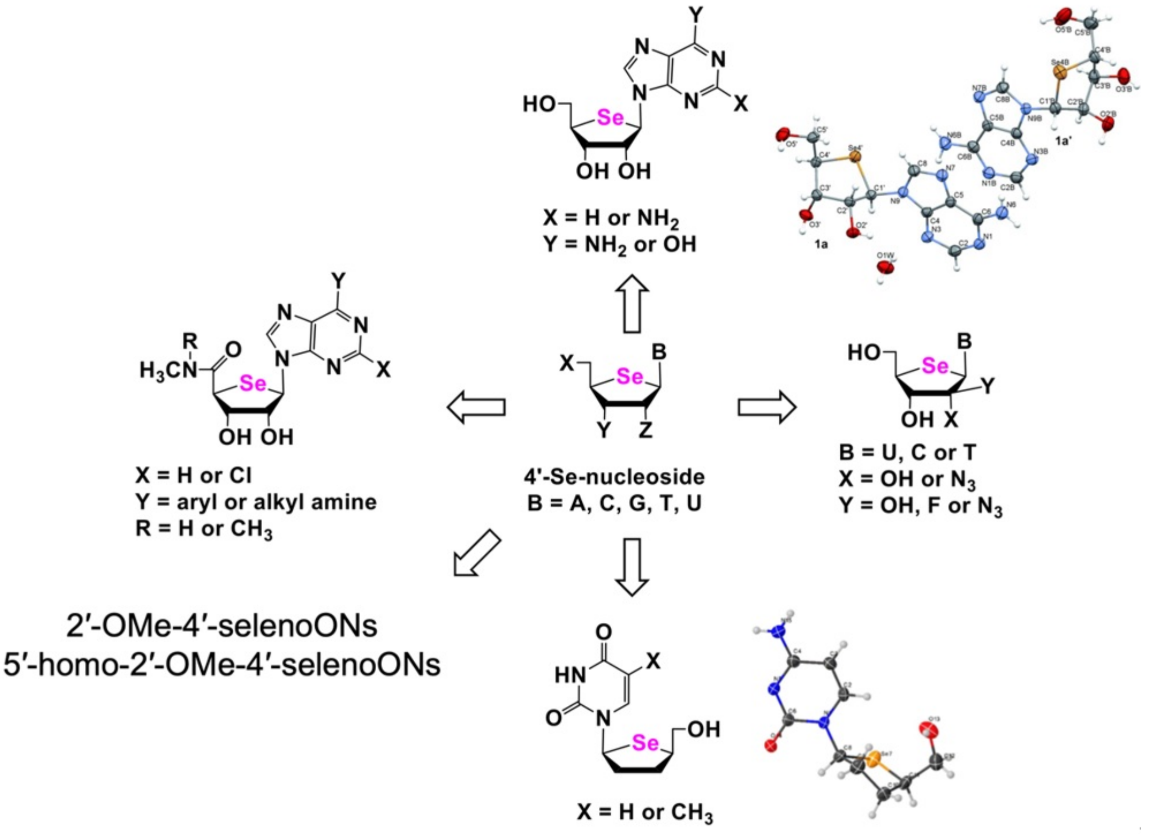
Symposium : **MEDI2-1**
Recent Trends in Drug Discovery Based on Nucleosides and Nucleic Acids
Room 301+302 FRI 09:00
Chair: Ki Tae Kim (Chungbuk National University)

Exploring the Therapeutic Potential of Modified Nucleosides, including 4´-Selenonucleosides

Jinha Yu

College of Pharmacy and Graduate School of Pharmaceutical Sciences, Ewha Womans University, Korea

Our research focused on the synthesis and biological evaluation of selenonucleosides, particularly the derivatives at the 4´-position of the sugar ring, where selenium replaces oxygen. We innovated a novel synthesis method for these 4´-selenonucleoside derivatives and determined their structures using x-ray crystallography. Our findings reveal that 4´-selenoadenosine derivatives serve as effective A3 adenosine receptor agonists, with the potential to address diseases related to this receptor. Moreover, the 4´-selenopyrimidine derivatives exhibited substantial anticancer activity, indicating their promise for anticancer drug development. Additionally, the oligonucleotides we synthesized, which include 4´-selenouridine, were assessed for thermal stability and resistance to nuclease degradation. This study broadens the scientific understanding of 4´-selenonucleosides and highlights their viability as therapeutic agents.


X = H or NH_2
Y = NH_2 or OH
1a
1a'
X = H or Cl
Y = aryl or alkyl amine
R = H or CH_3
4'-Se-nucleoside
B = A, C, G, T, U
B = U, C or T
X = OH or N_3
Y = OH, F or N_3
2′-OMe-4′-selenoONs
5′-homo-2′-OMe-4′-selenoONs
X = H or CH_3

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **MEDI2-2**
Recent Trends in Drug Discovery Based on Nucleosides and Nucleic Acids
Room 301+302 FRI 09:30
Chair: Ki Tae Kim (Chungbuk National University)

A novel mRNA platform utilizing modified nucleotides

Young Jun Seo

Department of Chemistry, Jeonbuk National University, Korea

The development of mRNA vaccine platform has been pursued through research aimed at regulating excessive immune responses to mRNA vaccines, inducing efficient interaction with antigen protein translation initiators, or enhancing the in vivo stability of mRNA platform to increase antigen protein expression. In terms of regulating excessive immune responses, methods utilizing modified nucleotides may be employed, while for efficient interaction with translation initiators, modification of the 5' Cap structure of mRNA constructs has been predominantly used. Additionally, research on the stability of mRNA constructs has been conducted by modifying the 3' end. The structural modification of mRNA using modified nucleotides, particularly, has been known to have significant impacts on direct regulation of excessive immune responses and antigen protein expression, serving as the key technology of Moderna and Pfizer vaccines. Therefore, our research team aimed to develop mRNA constructs incorporating new modified nucleotides to enhance antigen protein expression efficiency. Furthermore, regarding the regulation of expression by binding translation initiators, current mRNA platform utilize dinucleotide or trinucleotide-based capping materials for the 5' cap, and our research team conducted studies on developing a new cap 1-based mRNA platform to regulate antigen protein expression. Additionally, in our research on the stability of mRNA constructs, we introduced various modified nucleotides at the 3' end of mRNA platform to regulate antigen protein expression.

Symposium : **MEDI2-3**

Recent Trends in Drug Discovery Based on Nucleosides and Nucleic Acids

Room 301+302 FRI 10:00

Chair: Ki Tae Kim (Chungbuk National University)

Therapeutic Development using Chemically Modified Asymmetric siRNAs

Dong-ki Lee

Department of Chemistry, Sungkyunkwan University, Korea

Small interfering RNAs (siRNAs) are rapidly emerging as the third-generation therapeutics development platform with the capability to target virtually any disease-causing genes present in human genome. We have developed asymmetric siRNA (asiRNA) structures, wherein the sense strands are shorter than conventional siRNAs, and demonstrated that the asiRNAs show comparable target gene silencing activity with reduced non-specific effects. To make asiRNA-based therapeutics, we have introduced various chemical modifications in sugar and backbone structure of RNA, along with conjugation of delivery moieties such as lipids and N-acetylglactosamine (GalNAc) to generate cp-asiRNA and GalNAc-asiRNA, respectively. In this presentation, I will summarize our asiRNA platform for therapeutics development and the pre-clinical and clinical data based on this highly efficient and versatile drug development platform.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **MEDI2-4**

Recent Trends in Drug Discovery Based on Nucleosides and Nucleic Acids

Room 301+302 FRI 10:30

Chair: Ki Tae Kim (Chungbuk National University)

Precise Genome Engineering: from Nucleus to Mitochondria

Kayeong Lim

Brain Science Institute, Korea Institute of Science and Technology (KIST), Korea

The development of genome engineering tools has revolutionized the ability to directly target and modify genomic sequences in various organisms. Among these tools, base editing has emerged as a breakthrough technology that can induce point mutations at target sites without generating double-strand DNA breaks. Base editors enable efficient C-to-T or A-to-G conversions in cell lines, animals, and plants, offering great promise for correcting pathogenic mutations in gene therapy and studying the functional effects of single-nucleotide polymorphisms. In particular, the recently developed mitochondrial base editing strategy has broad implications for studying and treating mitochondrial diseases. Here, I will discuss novel methods for precise base editing in nuclear and mitochondrial DNA, using recombinant fusion proteins of programmable DNA-binding proteins and deaminases. To address critical issues for therapeutic use, base editing has the potential to improve its specificity and versatility.[Keywords: Genome engineering, Base editing, Mitochondrial DNA editing, Programmable deaminases]

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **MAT1-1**

Current Trends in Materials Chemistry for Electrochemical and Photochemical Catalyst

Room 407+408 THU 15:30

Chair: Myung Jun Kim (Sungkyunkwan University)

Single-Walled Zeolite Nanotubes: Discovery, Structure, Application

Christopher W. Jones

School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, United States

Synthesis of zeolites with hierarchical porosity that allow micropore access to a wider range of molecules has been a recent research focus. Early approaches included post-synthesis treatments to etch mesopores into zeolite crystals. More recently, new SDAs have been used to create 2D zeolite nanosheets interspersed by mesoporous regions, yielding nanosheets of several zeolitic topologies such as MFI, FAU, AEL and MWW. Here we describe the first synthesis and structural characterization of a quasi-1D hierarchical zeolite, specifically a single-walled nanotube that has a microporous zeolitic wall enclosing a central mesoporous channel [1]. Use of the novel structure for CO_2 capture from simulated flue gas and air will be described [2].

References

[1] Korde, A., Min, B., Kapaca, E., Knio, O., Nezam, I., Wang, Z., Leisen, J., Yin, X., Zhang, X., Sholl, D. S., Zou, X. Willhammar, T., Jones, C. W., Nair, S., Single-Walled Zeolite Nanotubes. Science (2022) 375, 62.

[2] Short, G.N., Burentugs, E., Proaño, L., Moon, H.J., Rim, G., Nezam, I. Korde, A., Nair, S., Jones, C.W. Single-Walled Zeolitic Nanotubes: Advantaged Supports for Poly(ethylenimine) in CO2 Separation from Simulated Air and Flue Gas. JACS Au (2023) 3, 62-69

Symposium : **MAT1-2**

Current Trends in Materials Chemistry for Electrochemical and Photochemical Catalyst

Room 407+408 THU 16:10

Chair: Myung Jun Kim (Sungkyunkwan University)

A step forward for better electrocatalysis through understanding of interfacial chemistry

Chang Hyuck Choi

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

Electrocatalysis at the electrode-electrolyte interface is fundamentally governed by electron transfer across the electric double layer (EDL), highlighting a critical mechanistic link between electrocatalytic properties and EDL structure. A key question in this field is the role of alkali metal cations at this interface, commonly referred to as the "cation effect". In this presentation, I will outline our ongoing research aimed at uncovering the fundamental principles underlying the cation effect on several important electrochemical reactions in aqueous environments. Using advanced in situ analytical techniques, we have begun to understand that the alkali metal cation is not merely a spectator, as traditionally assumed, but actively influences the kinetics and mass transport in electrocatalysis. The identity and concentration of the alkali metal cation are found to be critical not only in modulating electrocatalytic activity and selectivity, but also in influencing electrode stability. We will present potential mechanisms, including cation-coupled electron transfer, supported by experimental evidence. By gaining a deeper understanding of how alkali metal cation affects electrocatalysis, we aim to discuss and propose a novel conceptual framework for improving electrocatalytic processes.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

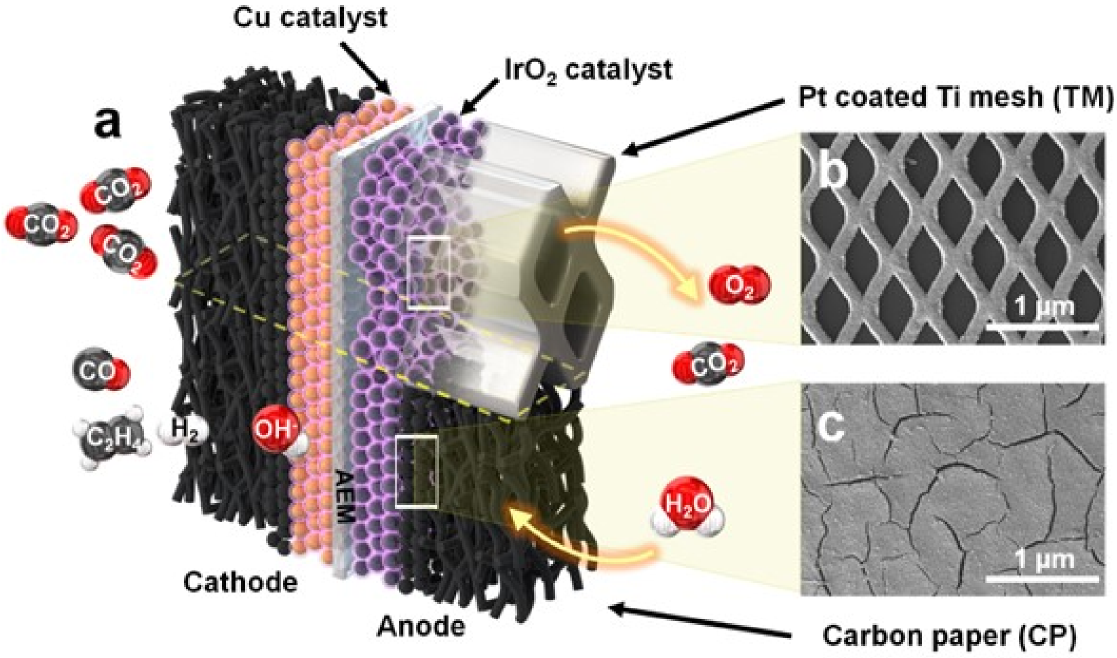
Symposium : **MAT1-3**
Current Trends in Materials Chemistry for Electrochemical and Photochemical Catalyst
Room 407+408 THU 16:35
Chair: Myung Jun Kim (Sungkyunkwan University)

e-Chemical production by CO_2 electrolysis

Hyung-Suk Oh

Clean Energy Research Center, Korea Institute of Science and Technology, Korea

Nanoscale catalytic materials are key components of various electrochemical devices for storing and converting renewable energy, such as fuel cell, water splitting and CO_2 electrolysis system. Their successful development and optimization require insight into the relations between atomic-scale structure of the catalytic interface and their electronic structure to improve the catalytic activity and stability. In this talk, we will highlight some of our recent work on the design and understanding of precious/non-precious metal and metal oxide catalyst materials for oxygen evolution reaction (OER) and CO_2 reduction reaction (CO_2RR). Especially, their electronic structure and electrochemical stability during operating condition were analysed by using in-situ/operando X-ray absorption spectroscopy. Based on these results, we will outline the preparation, characterization, and catalytic performance of metal and metal oxide model catalysts and discuss fundamental aspects of their structure-activity and –stability relationships.


Cu catalyst
IrO$_2$ catalyst
Pt coated Ti mesh (TM)
a
b
c
CO$_2$
CO$_2$
CO$_2$
CO
C$_2$H$_4$
H$_2$
OH$^-$
AEM
O$_2$
CO$_2$
H$_2$O
1 µm
1 µm
Cathode
Anode
Carbon paper (CP)

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **MAT1-4**

Current Trends in Materials Chemistry for Electrochemical and Photochemical Catalyst

Room 407+408 THU 17:00

Chair: Myung Jun Kim (Sungkyunkwan University)

Role of Interfacial Species in Electrochemical H_2O_2 Production

Young Jin Sa

Department of Chemistry, Kwangwoon University, Korea

Electrochemical production of H_2O_2 from the 2-electron oxygen reduction reaction ($2e^-$ ORR) is a promising alternative to the traditional anthraquinone process. For efficient H_2O_2 electrosynthesis, side reactions such as $4e^-$ ORR and H_2O_2 reduction, which are thermodynamically preferred, should be kinetically suppressed. In this regard, the development of active and selective electrocatalysts for the $2e^-$ ORR has been pursued. The electronic and geometric structures of catalytic active sites determine the adsorption properties, and thus activity and selectivity according to Sabatier principle. Besides the active site structures, chemical species at the catalyst-electrolyte interface can interact with the active sites and reaction intermediates, as well as modify the local mass transport and electron transfer properties; however, the role of interfacial species has rarely been understood.In this presentation, I will demonstrate two examples where the interfacial species improve the H_2O_2 electrosynthesis activity of carbon nanomaterials and suggest their possible roles. First, the type and concentration of alkali cations in electrolytes significantly influence the $2e^-$ ORR activity of surface-treated carbon blacks. The alkali cations affect the hydrogen bonding networks of the interfacial water molecules, and in turn, the rate of outer-sphere electron transfer, which has been suggested as the rate-determining step for the $2e^-$ ORR. Second, cerium oxide-carbon nanotube (CeO_x/CNT) hybrids are examined as the $2e^-$ ORR electrocatalysts and the role of interfacial CeO_x, as a surface promoter, is scrutinized.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **MAT2-1**
Emerging Semiconductors for Electronic Applications
Room 407+408 FRI 09:00
Chair: Hongje Jang (Kwangwoon University)

Composition and Ligand Engineering of Metal Halide Perovskite Nanocrystals for Efficient and Stable Light-Emitting Diodes

Seon Joo Lee*, Jaemin Lee[1]

Korea Research Institute of Chemical Technology, Korea
[1] *Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

In recent times, metal halide perovskite nanocrystals have emerged as a prominent choice among emissive materials, poised to steer the next-generation display industry. Lead halide perovskite nanocrystals (PeNCs) offer notable advantages such as a narrow full width at half maximum (FWHM), high photoluminescence quantum yields (PLQYs), and straightforward fabrication processes. These intriguing characteristics have led to the development of highly efficient PeNCs-based light-emitting diodes (PeLEDs) with impressive external quantum efficiencies (EQEs) as highlighted by various studies. Nevertheless, the stability of PeLEDs remains a concern due to the rapid degradation of PeNCs.In this presentation, I would like to discuss strategies for controlling the composition and ligands of PeNCs to achieve efficient and stable PeLEDs. We successfully incorporated sizable organic cations into the cesium-based PeNCs using room-temperature synthesis, as evidenced by XPS and FT-IR analysis. Additionally, by introducing ligands of the phosphonic acid, we were able to obtain stable uniform-sized PeNCs. The photoluminescence quantum yield (PLQY) of the optimized PeNCs reached over 90%. The thin film of the PeNCs exhibited enhanced stability when exposed to ambient conditions. We clarified the interactions between phosphonic acid ligands and the PeNC surface using P-NMR and XPS analysis.

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Symposium : **MAT2-2**
Emerging Semiconductors for Electronic Applications
Room 407+408 FRI 09:30
Chair: Hongje Jang (Kwangwoon University)

Electrolyte-Gated Transistors in Biosensor Applications for Early Disease Diagnosis

Young-Geun Ha

Department of Chemistry, Kyonggi University, Korea

Electrolyte-gated transistor (EGT)-based biosensors, which convert the presence or concentration of specific biological analytes into electrical signals, have attracted much interest because of their several advantages, including rapid label-free biomolecule detection, miniaturization for point-of-care applications, and integration with advanced electronics. In this presentation, I will explore both the fundamental and applied aspects of EGTs, as well as their use in novel applications such as biosensors to detect ultralow concentrations of target biomolecules, thereby facilitating early disease diagnosis. The first section will introduce a highly effective and efficient electrode passivation method using a facile solution-processed self-assembled multilayer (SAML) with excellent insulation properties to achieve operational stability and reproducibility of EGT biosensors. In the second section, I will describe rationally designed EGT biosensors with scalable grooved nanostructured oxide semiconductors fabricated by thermal nanoimprint lithography to overcome Debye length limitations for ultrahigh-sensitive biosensor applications. Overall, this presentation will offer an overview of EGT's applications in biosensors, highlighting its potential as a versatile tool in the early detection of disease.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Symposium : **MAT2-3**
Emerging Semiconductors for Electronic Applications
Room 407+408 FRI 10:00
Chair: Hongje Jang (Kwangwoon University)

Oxide Memristor Research for Bio-inspired Computing Applications

Jung Ho Yoon

Advanced Materials Science & Engineering, Sungkyunkwan University, Korea

Memristive devices have become a promising candidate for energy-efficient and high-throughput unconventional computing, which is a key enabler for artificial intelligent systems in the big data and IoT era. The so-called neuromorphic computing can be implemented on a resistive neural network with memristive synapses and neurons. In this talk, I will first briefly introduce memristive devices. I will then discuss the promises and challenges, including uniformity issues, non-linearity, and 3d structure compatibility, of the memristive devices & arrays, and also some approaches to overcome such issues. A few examples selected from our recent experimental demonstrations of the promising applications from next-generation memory to bio-system emulator, which utilize such memristors, are also introduced.

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Symposium : **MAT2-4**
Emerging Semiconductors for Electronic Applications
Room 407+408 FRI 10:30
Chair: Hongje Jang (Kwangwoon University)

Designer electronic materials for soft electronics

Jiheong Kang

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

In this presentation, I will first show my approaches to toughen self-healable network to use for soft electronic applications. The toughened self-healing materials realize exceptional mechanical properties such as notch-insensitive high stretchability, high toughness of 12,000 J/m^2, and autonomous self-healing even in aquatic environment. Second, I will talk about how to impart electronic functionalities to self-healable polymer network using nanomaterials. This approach is based on my recent finding that conductive nanostructured network can be reconstructed when it is surrounded by dynamic self-healing polymer matrix. Based on this self-healable conductive material, I was able to fabricate various functional electronic devices (ECG, EMG sensor, Display) and integrate them in a single platform capable of monitoring physiological signals and displaying feedback information through closed-loop communication between the user and electronics. Advantages of self-healable materials in the fabrication process at a system level will be discussed as well. Finally, I will show unexplored opportunities in interconnection technologies in soft electronics by the use of self-healable materials, which allow the users to design and construct their own electronics by simply cutting and pressing the robust, self-healable electronic modules (modular and reconfigurable electronics). Through my presentation, I will cover from fundamental development of self-healing materials to their system level applications in soft electronics.

Symposium : **MAT3-1**

Current Trends in Materials Chemistry for Porous Materials

Room 407+408 FRI 14:30

Chair: Seok Min Yoon (Gyeongsang National University)

Supporting Metal Nanoparticles within Zeolites and Their Analogues

Changbum Jo

Center for Nanomaterials and Chemical Reactions, Inha University, Korea

Transition metals are typically supported on a high surface area of porous materials to achieve a highly dispersed state, which is desirable for better utilization of the expensive metals. Typically, the highly dispersed state is thermodynamically unstable and tends to undergo sintering into large particles over time under harsh reaction conditions, resulting in the loss of catalytic activity. To minimize the deactivation, several strategies have been devised, including the immobilization of metal clusters onto the support surface via strong metal-support interactions and post-coating the metal nanoparticle with a shallow porous shell. Supporting metal clusters in the microporous channels or cavities can be an alternative strategy to obtain sinter-resistant catalysts when the microporous structure is stable under reaction conditions. Of the microporous supports, zeolite, a family of crystalline aluminosilicates, is an ideal scaffold due to its well-defined microporous and rigid network, high thermal stability, and capability of possessing acid sites in the framework. In my talk, I will introduce recent efforts to achieve zeolite-encapsulated catalysts, including the addition of organic ligands into the synthetic gel, kinetic control of zeolite crystallization, and the use of metal-containing zeolites as the seed. Then, I will present our strategy for metal encapsulation, using rationally designed organic molecules.

Symposium : **MAT3-2**

Current Trends in Materials Chemistry for Porous Materials

Room 407+408 FRI 15:00

Chair: Seok Min Yoon (Gyeongsang National University)

Hollow Metal Ceramic Electrocatalysts for Enhanced Ammonia and Hydrogen Production

Haneul Jin

Department of Energy and Materials Engineering, Dongguk University, Korea

Electrocatalysis, a surface-confined process, requires a comprehensive understanding of reactant and product adsorption and desorption phenomena on electrocatalysts. The surface characteristics, including surface energy, are intricately governed by atomic configurations within the surface and sub-surface layers of catalytic materials. Hollow/open structures have emerged due to their advantages in large specific surface areas and facilitated mass transports through the porous nanoshell, enhancing electrocatalytic performances. In this study, we present multi-metal ceramic-based electrocatalysts with hollow shapes, specifically designed for efficient water dissociation, resulting in the production of ammonia and hydrogen. Initially, we elucidate the synthesis process of Ir-doped Cu1.81S nanoparticles, exploring the impact of the dopant on electrochemical ammonia production effectiveness and mechanism. Subsequently, we introduce Pt and Ru-based phosphide nanocatalysts optimized for superior hydrogen production under alkaline conditions. The characterizations using transmission electron microscopy (TEM), cyclic voltammetry (CV), and density functional theory (DFT) calculations provide valuable insights into the physical and electrochemical properties of hollow structured multi-metal ceramic-based electrocatalysts.

Symposium : **MAT3-3**

Current Trends in Materials Chemistry for Porous Materials

Room 407+408 FRI 15:30

Chair: Seok Min Yoon (Gyeongsang National University)

Inorganic defective architectures for environmental sustainability disruptors remediation

Youngtak Oh

Center for Sustainable Environment Research, Korea Institute of Science and Technology (KIST), Korea

Humanity is facing the inevitable climate changes that endanger environmental sustainability. The excessive accumulation of atmospheric CO2, uncontrolled spread of radionuclide species, and the evolution of various toxic air substances put a heavy burden on the natural balance of the ecosystem. Here, my research group is devoted to developing new functional inorganic materials for various environmental remediation functions. Specifically, we have utilized various active defective sites within chalcogenides, carbon nanostructures, metal-organic heterostructures, and metal-oxide supported transition metal compounds in the form of aerogels, fibers, or nanoparticles. Through these architecture-driven adsorption or catalytic reactions, the diverse environmental remediation potentials for sustainable CO2 capture, aqueous radionuclide adsorption, and VOC conversion have been successfully demonstrated.

Symposium : **MAT3-4**

Current Trends in Materials Chemistry for Porous Materials

Room 407+408 FRI 16:00

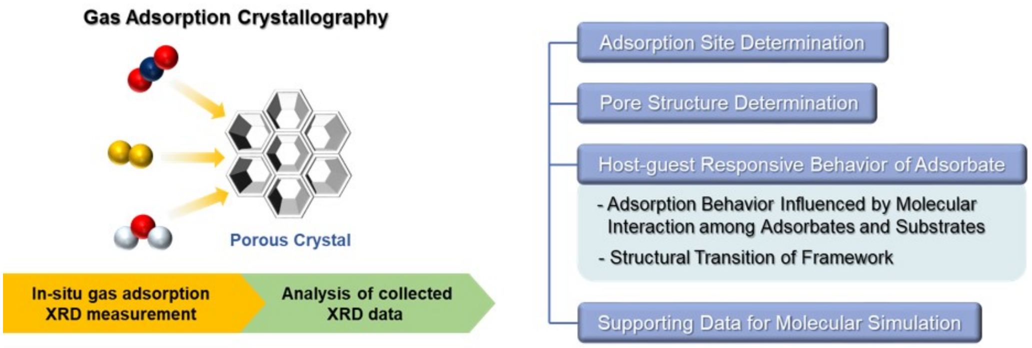
Chair: Seok Min Yoon (Gyeongsang National University)

Understanding adsorption of functional porous materials

Hae Sung Cho

Department of Chemistry, Chung-Ang University, Korea

Gas adsorption isotherm is one of general approach to characterize porous materials and develop their applications, but it does not directly give critical information concerning the adsorption behavior of gases in porous materials even they provide knowledge of the overall gas uptake within a material. To solve this limitation, X-ray diffraction (XRD) coupled with gas adsorption measurements (in-situ gas adsorption XRD) has been developed, which can serve the information about total electron charge distribution, positions and numbers, contributed from both adsorbates and the crystal. In this presentation, I will demonstrate the approach involving the measurement and analysis of in-situ gas adsorption XRD data, termed as “gas adsorption crystallography”, and show how the interactions among adsorbates and substrate, controlled by the pore environment and species of adsorbates, influence on the adsorption behavior. These works conclusively lead to a rigorous physicochemical understanding of the adsorption behavior, which can help to design of adsorbents with guest selectivity and uptake capacity.



Symposium : **ELEC1-1**

Research Progress in Stable Electrolyte/Electrode Interface for Energy Storage Systems

Room 105+106 THU 15:40

Chair: Seung Joon Yoo (GIST)

Interface Adhesives for Battery Electrodes

Jaegeon Ryu

Department of Chemical and Biomolecular Engineering, Sogang University, Korea

Rechargeable batteries have greatly advanced over the decades in terms of electrode host materials such as anodes and cathodes along with engineered electrolytes. Accordingly, unexpected issues occur at the electrode-electrolyte interface mainly related to the structural changes of host materials or (electro-)chemical instability of interface films, i.e. solid-electrolyte-interphase (SEI) layer. In this context, interface adhesives, also known as battery binders play a critical role in stabilizing the structure of large-volume-change host materials thereby securing or forming a stable SEI layer. However, such an adhesive layer needs to be designed taking the intrinsic surface property or lithium activity of host materials into consideration. In this presentation, the rational design of interface adhesives for various battery electrodes is discussed for the development of high-energy-density LIBs.

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Symposium : **ELEC1-2**
Research Progress in Stable Electrolyte/Electrode Interface for Energy Storage Systems
Room 105+106 THU 16:05
Chair: Seung Joon Yoo (GIST)

Design and analysis of advanced electrolytes for low temperature and fast charging lithium-ion batteries

Dong-Joo Yoo

School of Mechanical Engineering, Korea University, Korea

Since the commercialization of lithium-ion batteries (LIBs), it has made an impact on our society providing tremendous freedom of mobility. LIBs have been a key device not only in portable electronics such as smart phone, smart watch, or laptop, but also in applications for environmentally harsh conditions such as drone, space exploration, or defense equipment. While LIBs are required to be improved in many aspects of performance for those applications, low temperature capability is the most challenging one because the commercial electrolytes cannot operate properly at low temperature or high current density due to sharp drops in capacity and rate capability.LIBs have intrinsically slow kinetics at interfaces and bulk materials in both anode and cathode at low temperature, because Li ions have insufficient thermal energy for ion transfer at the interfaces and ion diffusion within bulk active materials to supply the required current density normally used during charge and discharge at room temperature. These impedances contribute to a large overpotential, resulting in a limited capacity and energy density at low temperature. In addition, the large overpotential during charging at graphite causes Li plating which impairs the cell performances and increases the safety issues with short-circuit. Furthermore, since there are many factors affecting performances at low temperature such as the sort of active materials, electrolytes, or electrode configurations, it is hard to pinpoint and address the actual limiting factor. In this presentation, I'd like to introduce limiting factors in LIBs at low temperature or high current density and some electrolyte design strategies to improve the kinetics at the interfaces. Since the conventional carbonate solvents have relatively high melting points and induce high charge-transfer resistances to the batteries, fluorinated ester-based electrolytes with high ionic conductivity and low interface resistance are

proposed and analyzed, giving a useful guideline in designing new electrolytes to address the low temperature and fast charging issues.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Symposium : **ELEC1-3**

Research Progress in Stable Electrolyte/Electrode Interface for Energy Storage Systems

Room 105+106 THU 16:30

Chair: Seung Joon Yoo (GIST)

Interfacial chemistry for advanced lithium metal batteries

Hee-Tak Kim

Department of Chemical and Biomolecular Engineering, KAIST, Korea

In recent decades, electrochemical devices, including batteries, fuel cells, and electrolysis, have made significant strides. However, their progress is often hindered by various interfacial problems that are challenging to identify and address. Space charges, double layer charges, charge transfer, and mass transport intricately influence the performance and durability of electrochemical devices. The complexity of interfaces and the limited means available for characterizing interface structures often result in unresolved or overlooked interfacial issues. This seminar emphasizes the importance of interfacial engineering and provides a fundamental understanding of electrode/electrode, electrolyte/electrolyte, and electrode/electrolyte interfaces. Based on this understanding, case studies are presented to demonstrate how to leverage this knowledge and control interface structures for designing advanced electrochemical devices.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **ELEC1-4**

Research Progress in Stable Electrolyte/Electrode Interface for Energy Storage Systems

Room 105+106 THU 16:55

Chair: Seung Joon Yoo (GIST)

Different Surface Dynamics of LiCoO2 by Cathode Electrolyte Interface and Artificial Layer across Potential Conditions

Junyoung Mun

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

This study aims to investigate effective methods for addressing two primary surface challenges that occur at high voltage levels in the cathode material LiCoO2: electrolyte side reactions and irreversible phase changes. To protect the surface degradation, two common surface modifications are utilized, artificial coating of Al2O3 and the formation of a cathode electrolyte interface (CEI) using a lithium bis(oxalate)borate (LiBOB) electrolyte additive. It is found that the cause of LiCoO2 degradation at 4.2-4.6 V is mainly from side reactions; however, at high voltages (> 4.7 V), it is attributed to irreversible structural changes. While the electrolyte additive LiBOB fails to prevent phase changes, Al2O3 coating enhances high-voltage cycleability by including Al diffusion to the surface structure, forming a doping layer. Our study suggests that while SEI mitigates side reactions at low voltage, it is not effective in preventing phase changes; however, coating with a doping layer can suppress phase changes and boost high-voltage performance.AcknowledgeThis work was supported by the Technology Innovation Program (20010900) funded by the industry of Trade, Industry & Energy (MOTIE, Korea)

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **ELEC1-5**

Research Progress in Stable Electrolyte/Electrode Interface for Energy Storage Systems

Room 105+106 THU 17:20

Chair: Seung Joon Yoo (GIST)

Reshaping Li+ Microenvironment and Interfaces for Safer, Faster Charging Li-ion Batteries

Hongkyung Lee

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

Amidst the surging demand for battery-powered automobiles, it is crucial to tackle the safety risks of Li plating triggered by high cell polarization to achieve extremely fast charging (XFC) of Li-ion batteries. This talk will explore the impact of Li+ desolvation and solid-electrolyte interphase (SEI) chemistry on cell polarizations. Notably, we propose linear carbonate (LC)-based, LiPF6-concentrated electrolytes (LPCEs). In the LC family, dimethyl carbonate (DMC) is thermodynamically preferred to facilitate desolvation kinetics, thereby lowering the charge-transfer barrier at the graphite anode. For effective graphite passivation and faster Li+ diffusion crossing the SEI, fluoroethylene carbonate (FEC) can help build up a thin and fluorinated SEI and reinforce the XFC cycling stability of graphite||NMC622 full cells (3.0 mAh cm−2; N/P = 1.1), exhibiting 94.3% capacity retention over 500 cycles under a 10-min charging condition. The excellent XFC performance is practically validated using a 1.2 Ah pouch cell, which demonstrates three times higher capacity retention over 200 cycles while suppressing Li plating-triggered cell swelling compared to conventional electrolytes. Further, it will be discussed on the efficacy of localized high-concentration approach using linear hydrofluoroethers (HFE)-based diluents. The original solvation structure can be reconfigured by the sort of HFE owing to intermolecular attraction forces. Moving away from the LHCE concept, the molecular engineering of main solvent will be further proposed to push the limit of XFC over 10 C-rate (6-min charging time). Unraveling the cell polarization governed by electrolyte chemistry provides valuable insights regarding future electrolyte designs for improving the XFC capabilities of Li-ion batteries.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Symposium : **ELEC2-1**
Recent Trends in Fundamental Electrochemistry
Room 105+106 FRI 09:00
Chair: Seung-Ryong Kwon (Gyeongsang National University)

Nanoporous Electrochemistry

Je Hyun Bae

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

Nanoporous electrodes are representative electrode materials for diverse applications, such as energy conversion devices and sensors. Research in nanoporous fields has recently diverted from the electrochemical behavior caused by an enlarged surface area to that caused by a nanoporous structure. Studies related to nanoporous structural effects are particularly relevant to electrochemistry because the electrochemical behavior in a nano-confined space differs from that in bulk space. The nanoporous morphological effect in electrochemistry is called “nanoporous electrochemistry”. Our efforts to understand the electrochemical phenomena caused by nanoconfined space of nanoporous electrodes will be presented.

Symposium : **ELEC2-2**

Recent Trends in Fundamental Electrochemistry

Room 105+106 FRI 09:30

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Application of ionic complexes based on multivalent carbon dot anions in electrochemical systems

Hongchul Lim[*], **Tae Hyun Kim**[1,*]

Department of Fine Chemical New Material, Sangji University, Korea

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

Carbon dots (also called carbon quantum dots or graphene quantum dots, abbreviated C-dots), a class of carbon allotropes, have gained great attention in recent years because of their great application prospects in energy, catalysis, bioimaging, and nanomedicine. Generally, C-dots are zero-dimensional materials with sp2/sp3 hybridized carbon structures in the core and hydroxyl and carboxyl groups at the edges. In this talk, I will present our recent efforts on ionic complexes based on C-dots for application in electrochemical systems as supporting electrolytes and as anionic dopants. Nano-sized polyanionic C-dots prepared by the hydrothermal oxidation process of carbon nanofibers form ionic complexes with alkali cations such as Li+, Na+, and K+. Thus, these ionic complexes based on the C-dots exhibited low Coulombic energy, excellent thermal/electrochemical inertness, and decent ionic conductivity dissolved in aqueous and organic solvents. Using the synthesized ionic complexes, I will discuss the utilization of synthesized ionic complexes as electrode active materials for supercapacitors and electrochemical biosensors, as well as investigate their applications as supporting electrolytes for lithium-ion batteries and electrochromic devices.

Symposium : **ELEC2-3**
Recent Trends in Fundamental Electrochemistry
Room 105+106 FRI 10:00
Chair: Seung-Ryong Kwon (Gyeongsang National University)

Electrochemical Innovative Platform for Smart Farming: Ion Selective Electrodes

Yang-Rae Kim

Department of Chemistry, Kwangwoon University, Korea

In the realm of modern agriculture, precision and efficiency are paramount. Integrating electrochemical platforms offers a promising avenue for enhancing the productivity and sustainability of farming practices. I will focus on developing ion-selective electrodes (ISEs) within the context of smart farming. ISEs are crucial in monitoring systems, providing real-time data on critical ions for plant growth and soil health. We have engineered ISEs with enhanced selectivity, sensitivity, and stability through meticulous fabrication tailored to the specific ion species prevalent in agricultural environments. Moreover, my research delves into the practical implementation of these ISEs within innovative farming frameworks. Farmers can effortlessly monitor soil nutrient levels, detect potential nutrient deficiencies or imbalances, and optimize fertilization strategies by incorporating these electrodes into wireless networks. This proactive approach maximizes crop yields and minimizes resource wastage and environmental impact. Additionally, the scalability and cost-effectiveness of these electrochemical platforms render them accessible to farmers across diverse socio-economic backgrounds, fostering inclusive agricultural practices. By harnessing the power of electrochemistry, I can revolutionize agricultural practices, promoting sustainability, efficiency, and productivity in the face of evolving global challenges. This research paves the way for precision agriculture to become the cornerstone of food production, ensuring food security for future generations. This work was carried out with the support of Cooperative Research Program for Agriculture Science and Technology Development (Project No. PJ015725032024) Rural Development Administration, Republic of Korea.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **ELEC2-4**

Recent Trends in Fundamental Electrochemistry

Room 105+106 FRI 10:30

Chair: Seung-Ryong Kwon (Gyeongsang National University)

Development of real-world diagnostic devices using electrochemiluminescence analysis

Ik-Soo Shin

Department of Chemistry, Soongsil University, Korea

Biomarkers in the human body and complex matrices such as blood, urine, and tissues, are powerful aids in clinical diagnosis and treatment monitoring. The detection, identification, and quantification of these molecules can lead to the development of sophisticated methods and instruments for analyzing clinically useful biomarkers, but one of the main challenges is the ultra-low concentration (i.e., sub-picomolar). Various analytical methods, such as surface-enhanced Raman spectroscopy, amperometric detection using electrocatalyst, or inter- (or intra-) molecular optical energy transfer, have been proposed as ways to address these issues, but are still a technological distance away from commercialization in the real world. In this context, electrochemiluminescence (ECL) has appeared to be a leading transduction technique due to its optimal combination of electrochemical and spectroscopic methods (i.e., Roche's Elecsys, MSD's S-Flex). However, despite its high sensitivity, ECL remains challenging for point-of-care diagnostics due to its technological limitations. Recently, by discovering innovative bipolar electrode arrays and new materials, we have overcome these limitations of ECL technology and developed high-performance diagnostic devices that can be used directly at the patient's bedside or the point of care. In my talk, I will give a brief introduction to this.

Symposium : **EDU-1**

Current Trends in Chemistry Education

Room 404 THU 15:40

Chair: Wonho Choi (Sunchon National University)

Challenges of teacher training colleges following changes in educational paradigm during transition period

<u>Sung Geun Kim</u>

Cheongju National University of Education, Korea

Science education has played a particularly important role in helping our country grow from an underdeveloped country to an advanced country. However, it is not able to closely respond to rapid social changes such as the population cliff, changes due to advancements in science and technology such as artificial intelligence, and changes in education policies such as the high school credit system. The number of elementary school students is expected to decline by nearly 40% over the decade of the 2020s, and the decline in the number of middle school students is expected to continue in earnest from 2028. This decline in the school-age population is expected to further deepen the decline in the turnover rate of graduates from teacher training colleges into the teaching profession, which is still worsening. This situation may raise issues about the identity of colleges of education and colleges of education as teacher training institutions. So far, teacher training colleges have played a role in participation in curriculum policies and re-education of teachers. However, considering the nature of the transition period, a new outlook will be needed to improve the quality of our education by enhancing the function of more active teacher re-education and strengthening the function and role as a teacher training-re-education institution.

In addition, the high school credit system, which is currently being introduced and will be implemented from 2025, is an opportunity for a qualitative change in the content of more specialized science education beyond the existing framework of science education if professional responses are applied in earnest. Teacher training institutions can also lead the role of a science technology-science education integration platform that reflects the rapid changes in science and technology taking place in modern society in school education.

In a rapidly changing transition period, a task that must be actively considered in the roles of teachers' and colleges of education is the strengthening of educational policy functions. The responsibility of national curriculum policy has already been transferred to the National Education Committee. Although the promotion of the revised 2022 curriculum was carried out under the jurisdiction of the Ministry of Education, the National Education Committee, which later took charge of curriculum policy, has the nature of an organization with a much stronger governance function than the Ministry of Education, which is an administrative agency. A policy plan containing the vision and prospects of science education should be created through more active gathering and efforts of expert groups from teachers' and education colleges.

Proactive response as a teacher training institution to the population cliff, re-establishment of a more active role as a teacher retraining institution, role as a professional platform that can incorporate rapid changes in science and technology into school education, and active cooperation between experts to prepare a macro and systematic science education policy vision. are important tasks.

I propose agendas in the hope that meaningful discussions will take place regarding these issues.

Symposium : **EDU-2**

Current Trends in Chemistry Education

Room 404 THU 16:00

Chair: Wonho Choi (Sunchon National University)

Challenges and Responses in University Chemistry Education during an Era of Rapid Population Decline: The Case of Regional Private University

Jeongho Cha

Department of Chemistry Education, Daegu University, Korea

In Korea, the rapid decrease in the school-aged population is causing significant transformations, including in education. This crisis, initially surfacing at the kindergarten level, is extending to university education, signaling a shift in higher education. This presentation examines the challenges and responses faced by university chemistry education in this era, specifically at one regional private university. The discussion explores the unique challenges brought about by the demographic shift, such as implications on curriculum development. It then traces the strategies employed by the university in response, examining the effectiveness of approaches like curriculum redesign and faculty development programs. The presentation concludes with a reflection on these findings for university chemistry education in Korea. It aims to contribute to a comprehensive discussion on navigating the future of university chemistry education amidst the declining population.

Symposium : **EDU-3**

Current Trends in Chemistry Education

Room 404 THU 16:40

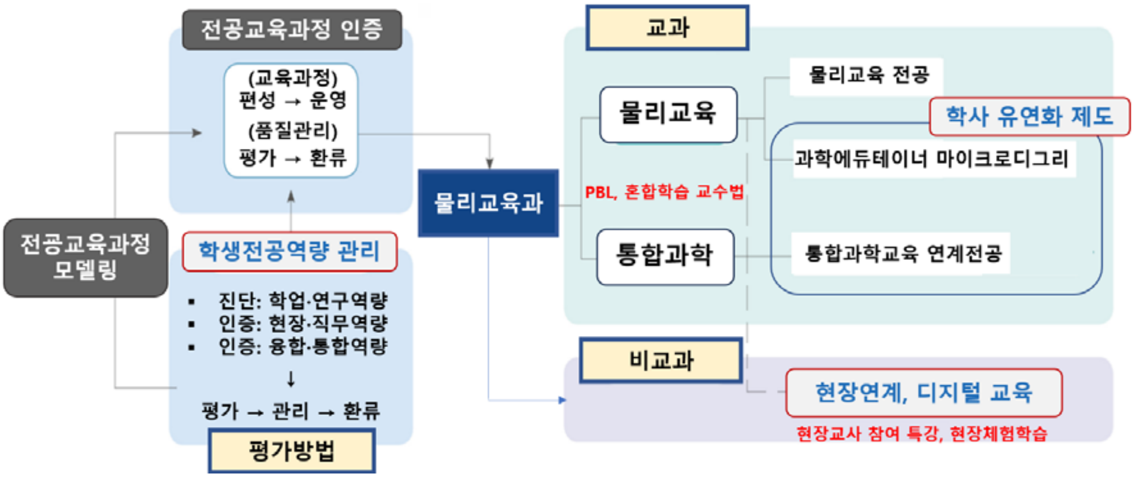
Chair: Wonho Choi (Sunchon National University)

Challenges and Responses of the Department of Physics Education for Career Diversification: The Case of a Regional National University

Jeongwoo Son

Department of Physics Education, Gyeongsang National University, Korea

Many people have recently predicted that the number of teachers will decrease due to the digital revolution, the decline in the school-age population, the high school credit system. Accordingly, our department has materialized its efforts to pioneer career paths other than teaching through the following process. First, we conducted major curriculum modeling and reorganized the curriculum. Based on environmental analysis and demand analysis, we set the department's educational goal. Moreover, we selected the ideal human resources as 'an educator of innovation and communication who leads future education.' Based on this, the subjects were classified into a major module course to become a physics teacher and physicist and a micro module course to become a science edutainer. In addition, a roadmap for course completion according to the student's career choice was created. Second, to increase the feasibility of the micro module, it was approved, opened, and operated as a micro degree curriculum. Third, various extracurricular activities, such as special lectures on digital education and visits to science museums, were operated to increase students' willingness to pursue career paths. Fourth, we conducted diagnostic evaluation and certification to manage students' major competencies according to these changes in the curriculum. We expect this result to appear in 2 to 3 years.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과학에듀테이너 마이크로디그리
통합과학교육 연계전공
비교과
현장연계, 디지털 교육
현장교사 참여 특강, 현장체험학습

133rd General Meeting of the Korean Chemical Society
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Symposium : **EDU-4**
Current Trends in Chemistry Education
Room 404 THU 17:00
Chair: Wonho Choi (Sunchon National University)

Concerns and alternatives on institution identity among research-oriented university and teacher training university in the era of population cliff

Dae Hong Jeong

Department of Chemical Education, Seoul National University, Korea

Currently, our country is facing a major social problem called the population cliff, and as a result, various problems are being revealed in each occupational group. In particular, the primary impact of the decrease in the number of students is a decrease in the number of teachers teaching in schools. Although the number of teachers may not decrease proportionally with the decrease in the number of students, it is accepted as a natural fact that the number of teachers decreases. For school levels that have not yet shown a decrease in the number of students, the government is preemptively reducing the appointment of new teachers by taking into account the teacher's working period. Accordingly, the concerns of teachers' colleges and universities, which are institutions that train teachers, not only deepened but also became a pressing issue.Seoul National University is a university that declares research-oriented university as its institutional identity, and the College of Education is an institution that defines teacher training as its institutional identity. In other words, the College of Education within Seoul National University has the obligation to pursue these two institutional identities. However, looking back on the history of the past 50 years, we see that these two identities are playing conflicting roles rather than coexisting. Undergraduate students enter after declaring their intention to become teachers, but the number of students who take the teacher appointment exam does not exceed 30%. In other words, if you think about it from the perspective of enrolled students, the majority of students choose a path other than that of a teacher while going through the four-year curriculum. This is where Seoul National University’s College of Education’s concerns begin. Although it fulfills its role as a teacher training institution, it provides education tailored to a small number of students, and the majority of students are finding other paths on their own. On the other hand, it is desirable for a research-oriented university that the majority of students choose academic follow-up courses rather than teacher courses, but it is true that most of them move to academic follow-up courses at other colleges rather than the academic follow-up courses at the College of Education. This points out the limitations of its role as a research-oriented university. Currently, the College of Education is collectively considering this issue in detail, and we believe that this issue may be partially related to other Colleges of Education, so we would like to have an open discussion together.

Symposium : **ENVR1-1**

Seawater Electrolysis Nexus Technologies

Room 403 THU 15:30

Chair: Hyunwoong Park (Kyungpook National University)

Multi-metal layered double hydroxides for alkaline oxygen evolution reaction under dynamic operation

MinJoong Kim

Korea Institute of Energy Research, Korea

Alkaline water electrolyzer (AWE) has the advantage of using low-cost electrode materials for the electrochemical water-splitting reactions. However, the sluggish kinetics of the OER limits its overall efficiency. Among many electrocatalysts, multi-metal layered double hydroxide (LDH) shows intrinsically better OER performance due to its layered structure, offering rapid diffusion of reactant, anion exchange, and hydroxyl adsorption. Until now, nickel-iron layered double hydroxide (Ni-Fe LDH) has been widely reported as the best OER catalyst for AWE. Despite its high OER activity, its poor operational stability remains an issue, as confirmed by various degradation studies. We aimed to overcome this issue by developing a highly durable electrode using the following two strategies.First, the approach to address the degradation issue initiated with density functional theory calculations, which proposed that the inclusion of a higher Fe content (>40%) than the theoretical Fe3+ limit (~25%) permitted by Ni-Fe LDH could improve its structural stability. Second, a customized galvanic cell has been developed based on corrosion principles to grow Ni-Fe LDH and Co-Fe LDH in Ni and Co salt solutions, respectively, on various substrates (Cu, Ni, Fe-Cr steel, and Ni-Fe-Cr steel). The practical feasibility of these LDH-based OER electrodes was demonstrated in a zero-gap type single-cell. This includes accelerated stress tests (AST), simulating on/off cycling, and fluctuating power supply protocols from solar and wind sources. These findings represent a crucial step towards developing reliable OER electrodes for commercial AWE systems, ultimately contributing to the broader goal of a sustainable energy future.

Symposium : **ENVR1-2**

Seawater Electrolysis Nexus Technologies

Room 403 THU 16:00

Chair: Hyunwoong Park (Kyungpook National University)

Electrolysis of seawater blended with wastewater for decentralized water reuse and hydrogen production.

Kangwoo Cho

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

The current societal pursuit towards carbon neutrality would necessitate self-contained systems, ultimately to be independent on the existing water and energy grid. On-site wastewater treatment and reuse can reduce water and waste transportation, in-turn decreasing the carbon footprint for sanitation and hygiene. Electrochemical oxidation processes (EOPs) have emerged as a promising way of decentralized treatment of toilet wastewater and effluent reuse. On the other hand, a distributed and point-of-use electrolysis of locally available, nontraditional water sources including wastewater (effluent) can be involved within the H_2 economy, reducing costs and CO_2 emission from H_2 transportation. This study proposes wastewater electrolysis cells (WECs) for localized wastewater treatment coupled with conversion of redundant renewable energy into H_2. In the single-compartment WEC, therefore, oxygen reduction reaction competes with the hydrogen evolution reaction (HER), substantially decreasing the current and energy efficiency. Relatively low-grade H_2 (< 60%) in mixture with N_2 and CO_2 can be utilized by combustion. This approach might be more available and appropriate practice in household and community level. This presentation also introduces recent electrocatalysts to overcome the bottlenecks of WEC such as requirements of precious elements based electrocatalysts and unsatisfactory selectivity of chlorine evolution reaction.

Symposium : **ENVR1-3**

Seawater Electrolysis Nexus Technologies

Room 403 THU 16:30

Chair: Hyunwoong Park (Kyungpook National University)

Atomically Dispersed Metal Catalysts Steering Selective Electrocatalysis of Chlorine Production

Sang Hoon Joo

Department of Chemistry, Seoul National University, Korea

The electrochemical chlorine evolution reaction (CER) is a key anodic reaction that has found wide utility in electrochemical industry. Since the 1970s’, Ru/Ti-based mixed metal oxides (MMOs) have been mainstays as a CER electrocatalyst. However, they suffer from the selectivity problem between the CER and parasitic oxygen evolution reaction (OER). Recently, we have developed a new CER electrocatalyst, atomically dispersed single site catalyst, which is high selective for the CER by breaking the scaling relationship between the CER and OER. This talk will present the discovery of atomically dispersed Pt sites on carbon nanotubes as a new CER electrocatalyst, its unusual CER kinetics and mechanism, and identification of its genuine active sites for the CER.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Symposium : **ENVR1-4**
Seawater Electrolysis Nexus Technologies
Room 403 THU 17:00
Chair: Hyunwoong Park (Kyungpook National University)

Seawater to Resource Technology using NASICON Solid Electrolyte

Youngsik Kim

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

Seawater serves as an abundant reservoir of valuable resources, encompassing substantial quantities of water and minerals. Nevertheless, the presence of diverse impurities in seawater impedes its direct utilization for resource extraction. To confront this challenge, an electrochemical approach employing a solid electrolyte termed NASICON (Sodium Super Ionic Conductor) presents efficacious remedies for extracting valuable resources from seawater. The NASICON ceramic functions as a robust barrier against impurities and facilitates the discerning transportation of Na+. In this study, we present a comprehensive scrutiny of NASICON ceramics, furnishing an overview of the concept and accentuating the competitive advantages of NASICON-based electrochemical systems: particularly in the domains of energy storage, hydrogen production, sodium hydroxide and chlorine synthesis, water treatment, and mineral extraction. Additionally, this investigation covers the principal challenges necessitating attention and explores the trajectory of its progression towards attaining maturity as a technology.

Symposium : **ENVR1-5**
Seawater Electrolysis Nexus Technologies
Room 403 THU 17:30
Chair: Hyunwoong Park (Kyungpook National University)

Desalination-coupled seawater electrolysis

Hyunwoong Park

School of Energy Engineering, Kyungpook National University, Korea

An enormous amount of seawater is considered an ultimate feedstock for large-scale on-site hydrogen production via electrolysis coupled with a renewable electricity grid. The electrolysis of seawater is challenging, particularly because chloride oxidation reaction (ClOR) competes with OER. To minimize the interfering ClOR, seawater has often been highly alkalinized by adding KOH or NaOH. Despite the selective process of the OER, the as-obtained H2 cost should be greater than that with natural seawater at pH ~8.2, owing to the use of expensive, corrosive hydroxide salts. In addition, alkaline earth metal hydroxides are readily formed on the cathode, where the local pH is higher than the bulk pH due to the interfacial HER. We propose the electrolysis of in-situ desalinated water with anion exchange, cation exchange, and bipolar membranes (BPMs). The proposed membrane-coupled electrolysis has various advantages. For electrolysis, we synthesized Ni- and Fe-layered double hydroxides (NiFe-LDH) and binary NiMo metals as OER and HER electrocatalysts, respectively. The as-synthesized NiFe-LDH and NiMo pair was equipped into the as-designed membrane cell arrays with saline water. All individual reactions (desalination, production of HCl and NaOH, OER, and HER) occurred successfully, with low overall specific energy consumption for desalination, while producing various value-added chemicals (H2, HCl, and NaOH).

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Symposium : **ENVR2-1**

Recent Advances in Closed-loop Waste Plastics

Room 403 FRI 09:00

Chair: Yosep Han (KIGAM)

Separation of waste PVC/PET plastics using froth flotation with selective modification

Seongsoo Han

Mineral Processing & Metallurgy Research Center, Resources Utilization Division, Korea Institute of Geoscience and Mineral Resources, Korea

Most household plastic waste, including PE, PP, PS, PET, and PVC, are thermoplastic materials that may be recycled at moderate temperatures without notable degradation, facilitating their recycling process. However, most of them are mixed and discharged without separation, making plastic recycling difficult. This is because the quality of the recycled product degrades as a result of the different chemical structures of mixed plastics introduced into the recycling process. In particular, it is very important to separate PVC from other waste plastics. In contrast to PET, PP, PS, and PE, which consist solely of carbon and hydrogen atoms, PVC contains chlorine (Cl), which, when incinerated, produces toxic byproducts including dioxin and hydrochloric acid. PVC is readily separated by water along the specific gravity line from PE, PP, and PS, which have specific gravities equal to or less than 1. PVC has a specific gravity of approximately 1.3. However, its separation from PET of comparable specific gravity proves to be challenging. Hence, this study was to employ flotation to separate PVC and PET. Flotation is a process that separates solid particles of one component from particles of other components by selectively adsorbing them to the interface (air-water, oil-water). Selective adsorption is governed by the interaction force between the interface and particles, with hydrophobic interaction constituting the predominant interaction. That is, hydrophobic particles are adsorbed to the interface of air bubbles or oil droplets and then floated, and hydrophilic particles are allowed to stay in water, which is a continuous phase, to separate the two particles. Tannic acid and methyl cellulose were used as selective surface modifiers for PET. And for PVC/PET separation through flotation, comprehensive influencing factors such as particle surface hydrophobicity and particle size were investigated. As a result, tannic acid showed the effect of a selective surface modifier, and when the average bubble size was less than 0.5 mm, it was possible to selectively separate PVC from PET. Finally, it was possible to control the bubble size and successfully separate PVC and PET from tannic acid.

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April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Symposium : **ENVR2-2**

Recent Advances in Closed-loop Waste Plastics

Room 403 FRI 09:30

Chair: Yosep Han (KIGAM)

Small water droplet removal from pyrolysis oil

Siyoung Choi

Korea Advanced Institute of Science and Technology, Korea

To effectively separate emulsions composed of fine, sparsely distributed droplets, traditional methods typically require a membrane with pores small enough to match or even be smaller than the droplets themselves. While this ensures high separation efficiency, it limits the technique's application to emulsions with comparatively large droplets. Overcoming this challenge often involves adding a secondary membrane to reduce pore size, a process that can be both complex and expensive. Addressing the need for a simpler, more cost-effective solution, our study introduces an innovative approach using a pre-wetted mesh membrane. Unlike conventional methods, the pore size of this membrane is significantly larger than the droplets it separates. Created by simply applying water to a hydrophilic stainless-steel mesh, this membrane achieves separation through gravity-driven flow. Remarkably, it maintains a separation efficiency of over 98%, even for droplets approximately ten times smaller than its pores, offering a promising new direction for emulsion separation technology.

Symposium : **ENVR2-3**
Recent Advances in Closed-loop Waste Plastics
Room 403 FRI 10:00
Chair: Yosep Han (KIGAM)

The policy and technical trend of incineration in waste plastic treatment for circular economy

Youngjae Kim

Inha University, Korea

Since the generation of dioxin in the incineration process was firstly reported in 1983, the incineration of waste-plastic in the municipal incinerator has been paid great attention. The exhaust gas treatment system has been improved and exhaust controls have been enacted. Now, in Korea, there is regulation of dioxin generation for the operation of municipal incinerator, and most of control standard is as stringent as European one. The waste plastic disposal processes can be categorized into three ways; energy recovery, incineration and recycling. In Korea, the incineration is about 33 % and it is ranked 2nd following the energy recovery. In this stage, the energy recovery does not mean the conversion of plastic into pyrolysis oil, but it means the generation of heat energy by incineration of plastic. That means, most of plastic is now consumed in the incinerator or several plant, such as cement kiln, as the heat source. However, the ministry of environment in Korea announced the increasing of recycling rate and pyrolysis oil production rate in near future. For this reason, the plastic sources for incineration process would be more complicated and low-graded. That means the regulations for toxic gas generation would become stricter and its operation condition would be newly proposed.

Symposium : **ENVR2-4**

Recent Advances in Closed-loop Waste Plastics

Room 403 FRI 10:30

Chair: Yosep Han (KIGAM)

Technology trends to establish a closed-loop system for upcycling of waste plastics: Physical treatment perspective

Yosep Han

Resource Utilization Division, Korea Institute of Geoscience and Mineral Resources, Korea

In recent years, there is an increasing interest in environmental friendly treatment of waste-plastics in terms of the generation of microplastics. Accordingly, the recycling/upcyciling of waste-plastics in very important because it provides advantage of volume reduction, carbon dioxide emission, and reproduction of value-added products. In particular, the development of effective separation methods is very important in terms of material recycling (i.e. mechanical recycling). Therefore, the research trend of flotation, gravity and electrostactic separation for effective physicochemical separation of mixture waste-plastics were investigated. In addition, this presentation intends to present an approach to establishing a closed system for the upcycling of waste plastics. (Acknowledgements: This work was supported by the National Research Council of Science &Technology (NST) grant by the Korea government (No. CCL22131-100))

133rd General Meeting of the Korean Chemical Society

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:00

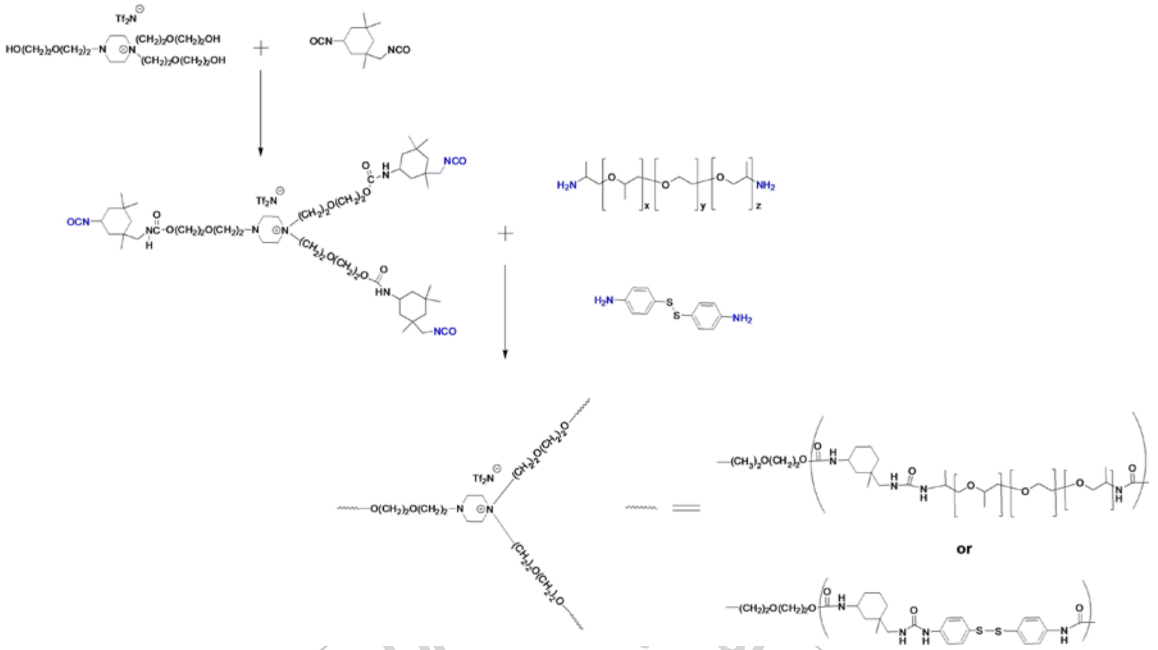
Chair: Byungjin Koo (Dankook University)

Synthesis and Characterization of a Cross-Linked Ionic Liquid Polymer Incorporating Piperazinium-Tf_2N

JongChan Shin, **Minjae Lee**[1,*]

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

Polymers based on ionic liquids are being recognized as promising candidates for polymer electrolytes due to their high ion conductivity and mechanical strength. However, there is a problem of low polymerization degree during the polymerization of ionic liquids due to the repulsion between the monomers of the ionic liquid. In this study, we synthesize piperazinium-based ionic liquid monomers with three or more polymerizable functional groups introduced for the formation of cross-linked polymers, aiming to achieve high mechanical strength in polymer-based on ionic liquids. To achieve various properties of polymers, cross-linked ionic polymers were synthesized using piperazinium salt monomer, jeffamine® and 4,4'-diaminodiphenyl disulfide in different ratios. The synthesized monomers and polymers underwent structural analysis using NMR and IR spectroscopy. Following this, the cross-linked ionic polymers were investigated for their crosslinking density based on the ratio of ionic monomers and co-monomers, followed by a characterization study. Furthermore, for application research as polymer electrolytes, thermal and electrical properties were studied by mixing them with Li salts. The detailed structures and properties of these materials will be discussed in the presentation.



Tf2N
HO(CH2)2O(CH2)2–N
(CH2)2O(CH2)2OH
(CH2)2O(CH2)2OH
OCN
NCO
H2N
NH2
x
y
z
S
or

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 09:15

Chair: Byungjin Koo (Dankook University)

Highly Effective Polymerization of Propylene Oxide and CO_2 Using Ultra Thin Zn-gallate

Kihyuk Sung, Hye-Young Jang[1,*]

Department of Energy Systems Research, Ajou University, Korea
[1]*Department of Chemistry, Ajou University, Korea*

Utilizing CO_2 as a carbon feedstock in polymerization processes offers a promising avenue for advancing sustainable chemical practices, expanding the range of plastic products capable of incorporating carbon dioxide. Despite extensive efforts to enhance catalytic performance, current methods employing zinc glutarate (ZnGA) as a heterogeneous catalyst for producing alternating polycarbonate from propylene oxide (PO) and CO_2 remain limited by relatively low activity (0.083 kg/g-cat). Addressing this challenge, we introduce a novel approach using Zn-gallate, a cost-effective catalyst synthesized from zinc salts and gallic acid without complex procedures. Zn-gallate exhibits exceptionally thin sheets (1–2 nm), delivering remarkable catalytic activity (3.01 kg/g-cat), high carbonate linkage proportion (f_{CO2} = 0.97), and selectivity (91%) in PO-CO_2 copolymerization, outperforming other zinc based heterogeneous catalysts. Moreover, synthesized polycarbonates from Zn-gallate demonstrated significantly elevated molecular weights. Comprehensive characterization via various analytical techniques provides valuable insights into the catalytic properties of Zn-gallate, elucidating its potential as a catalyst for sustainable polymerization processes.

Oral Presentation : **POLY.O-3**
Oral Presentation for Young Polymer Scientists
Room 303 THU 09:30
Chair: Byungjin Koo (Dankook University)

Anion exchange membrane with an interstitial alkyl chain in the conducting group and backbone for superior durability of water electrolyzer : from single cell to large cell stack

Haeryang Lim, Wooteak Jung, Taiho Park[1,*]

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

Anion exchange membrane water electrolysis (AEMWE) has garnered as an attractive alternative to alkaline water electrolysis and proton exchange membrane water electrolysis (PEMWE) due to its high efficiency and low hydrogen unit cost. However, the long-term durability of AEMWE is about 10-fold lower compared to the durability of PEMWE, which can typically operate 40,000 h. Herein, we report a novel design strategy for AEMs and synthesis an aryl ether-free PFPBPF-QA AEMs with interstitial alkyl chains in the conducting groups and polymer backbone. The rationally designed PFPBPF-4-QA exhibited mechanically robustness, alkaline stability, and high ionic conductivity, as well as stronger membrane-ionomer adhesion at CL. Thus, AEMWEs single cell using the PFPFTP-4-QA AEM exhibit a voltage decay rate of 2 mV kh^{-1} at 1.0 A cm^{-2}, which is much lower than other reported AEMWEs and Nafion-based PEMWEs. Moreover, a large sized 1-cell AEMWE stack with an active area of 63.6 cm^2 exhibited an energy conversion efficiency of 80.5% for 1000 h and voltage decay rate of 0.1 mV kh^{-1}, which can be expected to retain 90% of their initial efficiency after 1000 h of operation.

133rd General Meeting of the Korean Chemical Society
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Oral Presentation : **POLY.O-4**
Oral Presentation for Young Polymer Scientists
Room 303 THU 09:45
Chair: Byungjin Koo (Dankook University)

Designing Degradable Polymers from Tricycloalkenes via Complete Cascade Metathesis Polymerization

Tae-Lim Choi[*]**, Yongkang Yang**[1]

Division of Chemistry, Seoul National University, Korea
[1]*Department of Materials, ETH Zurich, Switzerland*

Cascade metathesis polymerization has been developed as a promising method to synthesize complex but well-defined polymers from monomers containing multiple reactive functional groups. However, this approach has been limited to the monomers involving simple alkene/alkyne moieties or produced mainly non-degradable polymers. In this study, we demonstrate a complete cascade ring-opening/ring-closing metathesis polymerization (RORCMP) using various tricycloalkenes and two strategies for the efficient degradation. Through rational design of tricycloalkene monomers, the structure and reactivity relationship was explored. For example, tricycloalkenes with trans configuration in the central ring enabled faster and better selective cascade RORCMP than the corresponding cis isomers. Also, a 4-substituted cyclopentene moiety in the monomers significantly enhanced the overall cascade RORCMP performance, with the maximum turnover number (TON) reaching almost 10,000 and molecular weight up to 170 kg/mol using an amide-containing monomer. Furthermore, we achieved one-shot cascade multiple olefin metathesis polymerization using tricycloalkenes and a diacrylate, to produce new highly A,B-alternating copolymers with full degradability. Lastly, we successfully designed xylose-based tricycloalkenes to give well-defined polymers that underwent ultra-fast and complete degradation under mild conditions.

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Oral Presentation : **POLY.O-5**
Oral Presentation for Young Polymer Scientists
Room 303 THU 10:00
Chair: Byungjin Koo (Dankook University)

Dynamic Crosslinking Effects on Thermal Behavior and Strain Sensitivity of CNT Composite Materials: A Systematic Analysis

Gyeonghyeon Choi, Chiyoung Park*

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

In this study, we conduct a comprehensive analysis of the thermal behavior of carbon nanotube (CNT) composite materials, focusing on dynamic crosslinking and filler concentration. Through meticulous rheological analysis across varying temperatures, we unravel the intricate relationship between crosslinking density and dynamic responsiveness within the composite materials. Our findings reveal that the thermal behavior of dynamic crosslinking governs the physical connectivity network of CNT fillers within the polymer matrix, consequently influencing key properties such as conductivity. Notably, CNT fillers are known for their outstanding thermal properties, particularly in the near-infrared (NIR) region under electrical excitation. Leveraging the correlation between crosslinking density and rheological characteristics established in this study, we demonstrate that higher crosslinking densities exhibit heightened levels of strain sensitivity, while also displaying nuanced responses to voltage, light wavelength, and intensity. Furthermore, our research underscores the ease of mechanical and chemical recyclability offered by dynamic crosslinking polymer network composite materials, along with their remarkable reproducibility of strain sensitivity post-recycling. This remarkable reproducibility is attributed to the preservation of network integrity during the recycling process, facilitated by the robust dynamic crosslinking. We anticipate that our findings will provide pivotal insights for both foundational and applied research in polymer and polymer-based conductive composite materials.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:15

Chair: Byungjin Koo (Dankook University)

Rational Design and Synthesis of Biodegradable Filler-Reinforced Networks for Superabsorbent Polymers

Young-Ho Kim, **Myungeun Seo***

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

The increasing demand for biodegradable materials in various fields has led to a growing interest in developing hydrogels derived from natural polymers. Chitosan, a biocompatible and biodegradable polysaccharide derived from crustacean shells, is a promising material for the synthesis of hydrogels. Chitosan hydrogels have been widely studied for tissue engineering, drug delivery, and wound healing. However, the synthesis method used to create these hydrogels also plays a critical role in their overall properties. Reversible Addition-Fragmentation Chain Transfer (RAFT) polymerization has been shown to be a suitable method for synthesizing chitosan-based hydrogels, as it allows for control over the molecular weight and the microstructure of the resulting hydrogel. This research aims to investigate the synthesis of biodegradable chitosan-based hydrogels by grafting from the chitosan backbone via RAFT polymerization. The chitosan also acts as a cross-linker, we anticipate that this design will allow us to have a larger mesh size and improve mechanical strength since the cross-linking sites are densely located at the chitosan backbone. By controlling monomer and chain transfer agent ratios, we explore the synthesized hydrogels' water swelling ratio and modulus.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:30

Chair: Byungjin Koo (Dankook University)

Topological Influence of Polyglycerols on Ice Recrystallization Inhibition Dynamics

Aram Shin, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

Antifreeze proteins protect organisms from freezing damage by inhibiting ice formation. Ice recrystallization inhibition (IRI) of various small molecules and polymers has been extensively investigated. In our previous research, we demonstrated the effect of branching degree on ice formation behavior including hyperbranched (hbPG) and linear polyglycerol (linPG) in a pure water environment. While this system posed a promise in regulating the ice recrystallization, it was limited to pure water system, which thus necessitates further development in biological system. Herein, we demonstrated a high IRI activity of dendritic polyglycerols (dPGs). Specifically, dPGs with different generations (dPG-2, dPG-3, and dPG-4) are prepared via iterative two-step reactions starting from trimethylolpropane and their IRI activity in biological buffer system was accessed. Interestingly, IRI activity of dPGs increased with increasing generation. Additionally, we investigated the ice growth rate of PGs through molecular dynamic simulations. Finally, cryopreservation using dPG-4 exhibited a better performance compared to the conventional 10% DMSO solution, posing a high potential in future cryopreservation agents.

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

Oral Presentation for Young Polymer Scientists

Room 303 THU 10:45

Chair: Byungjin Koo (Dankook University)

Homogeneous Macromolecular Networks by End-to-End Click Chemistry between Discrete Tetrahedral Star Macromolecules

Mo Beom Koo, Jae Hak Lee, HeeJeong Jang[1], Kyoung Taek Kim[2,*]

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

Homogeneous macromolecular networks were synthesized by end-to-end click chemistry between tetrahedral star macromolecules composed of PLA arms with defined molecular weights. The resulting polymer networks exhibited excellent degree of swelling in solvents without sacrificing their mechanical robustness, which could resulted from the minimal defects in the structures. To investigate the structural homogeneities of the networks, network disassembly spectroscopy was conducted by site-specifically breaking sequence-defined PLA chains between the cross-links, confirming that homogeneous polymer network with minimal defects were formed. Homogeneous networks of sequence-defined discrete tetrahedral star macromolecules could provide a rational way to precisely control the mechanical properties and chemical functionalities of polymer networks and hydrogels.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 405+406 THU 09:00

Chair: Jin Yeong Kim (Seoul National University)

Investigating the Thermoelectric Properties of Self-assembled Monolayers by Employing a Liquid Electrode

Sohyun Park

School of Chemistry and Energy, Sungshin University, Korea

Global warming is exacerbating, leading to an accumulation of excess heat on Earth. This waste heat can be converted into electricity through the thermoelectric phenomenon. However, the complicated molecular structures of active components and ill-defined interfaces of thermoelectric devices pose challenges for performance improvement. To enable practical applications of thermoelectric devices, the relationship between the chemical and electronic structures of active components and the thermoelectric performance of devices should be elucidated at a molecular scale.In this talk, I will present the development of a large-area thermoelectric measurement platform to measure the thermoelectric performance of a self-assembled monolayer and introduce the atomic-level structure-thermopower relationships found.

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 405+406 THU 09:15

Chair: Jin Yeong Kim (Seoul National University)

Bi- or multi-metallic complexes supported by a urea-backboned tetradentate [NNNN] ligand

Kyounghoon Lee

Department of Chemical Education and Research Institute of Natural Sciences, Gyeongsang National University, Korea

Multi-metallic complexes have shown unprecedented reactivity, such as small molecule activations and catalytic reactions based on metal-metal cooperativity. Integrating redox-active ligands that coordinate multi-metallic cores would be helpful, but only a few ligands have been reported. Here, we describe the synthesis of a urea-backboned tetradentate [NNNN] ligand (1) and its coordination chemistry to form bi- or multi-nuclear first-row transition metal complexes. Treatment of 1 with NiCl2(DME) (DME = dimethoxyethane) in the presence of two equivalents of NaOtBu formed a binuclear Ni(II) complex {(NNNN)Ni}2 (2). The same reaction using a weaker base NEt3 formed a cluster (MeO){κ3-H(NNNN)}3(NiCl)3Ni(NiCl)3{κ3-H(NNNN)}3(OMe) (3) where one equivalent of Cl- was eliminated with a concomitant deprotonation of 1. In addition, treatment of 1 with two equivalents of CuCl and two equivalents of NaOtBu formed a mixed-valent binuclear Cu complex Na{(NNNN)Cu}2 (4), presumably resulting from a disproportionation reaction. The characterization and applications of multimetallic complexes will be discussed.

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 405+406 THU 09:30

Chair: Jin Yeong Kim (Seoul National University)

Tuning Heterogeneous Catalysis Using Interfacial Polarization

Jaeyune Ryu

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

A plethora of the current energy conversion strategies hinge upon heterogeneous catalysis occurring at solid-liquid interfaces. Efficient heterogeneous catalysis requires control over inner-sphere bond activation and rearrangement reactions taking place at the solid catalyst surfaces. Thus, in addition to the active structure, the local microenvironment within molecular length scales of the catalyst surface defines reaction rate and selectivity. This local environment is radically different from the environment in the bulk of liquid phase because of the interfacial polarization that accrues from spontaneous and driven charge separation at the catalyst surface, generating a sharp electrostatic potential gradient and non-equilibrium concentration gradients. As such, a quantitative understanding of the polarization-induced interfacial local environment under reaction conditions is essential for understanding reactivity trends and for the rational design of new catalysts. Herein, we report the first localized measurements of electrostatic field strength and non-equilibrium concentration gradients within the electrical double-layer region during catalysis by utilizing a unique nonfaradaic molecular probe, which senses the localized proton activity within molecular length scales of the catalyst surface. Leveraging this fundamental knowledge of polarization-induced local environments at molecular length scales, we establish a general mechanistic framework for harnessing interfacial polarization to promote non-electrochemical heterogeneous catalysis under mild reaction conditions.

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 405+406 THU 09:45

Chair: Jin Yeong Kim (Seoul National University)

Expanding Heterobimetallic Catalysis: New Synthetic Model Complexes for Investigating Reactivity on Heterogeneous Surfaces

Dongyoung Kim, Yeong Jun Son, Seung Jun Hwang[1,*]

Chemistry, Pohang University of Science and Technology, Korea

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

A growing number of industrial heterogeneous reactions now depend on heterometallic systems. Frequently, at least two different metals with distinct properties contribute to unusual reactivity, catalyzing challenging chemical transformations. However, understanding the interactions between these metals that lead to such reactivity remains largely unknown and challenging to investigate due to limited spectroscopic tools for studying the reactive heterogeneous surface. Synthetic inorganic chemistry can offer a potential solution to gain this understanding. For example, creating synthetic analogs that mimic the ensemble of metals on heterogeneous catalysts can provide molecular-level insights by examining the electronic structure through various spectroscopic tools. To address this, we have developed a novel ligand system capable of hosting two pairs of metals, forming a tetrametallic molecular complex. As a case study, we employed this tetrametallic complex to explore the role of aluminum atoms in Cu/Al-based zeolites, which can catalyze the C–H bond activation of methane.

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Oral Presentation : **INOR.O-5**
Oral Presentation of Young Scholars in Inorganic Chemistry
Room 405+406 THU 10:00
Chair: Jin Yeong Kim (Seoul National University)

Two-Coordinate Au(I) Complexes for Highly Efficient Electroluminescence

Byung Hak Jhun, Youngmin You[1,*]

Department of Chemical and Biomolecular Engineering, Yonsei University, Korea
[1]*Chemical and Biomolecular Engineering, Yonsei University, Korea*

Two-coordinate complexes of coinage metals such as Cu, Ag, Au have emerged as promising alternatives to conventional late transition metal complexes. These novel complexes produce efficient light emission by harnessing ligand-to-ligand charge transfer to harvest triplet excitons, offering promising applications in bio-imaging, electroluminescence, and photocatalysis. We developed near-infrared (NIR)-emissive Au(I) complexes by controlling amido ligands. Our quantum chemical calculation and photophysical studies revealed the action of radiative control in the emergence of the NIR emission, which is parametrized from the distance between the hole centroid in the first singlet excited state and the nitrogen atom of the amido ligand ($d_{\text{h-N}}$).

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 405+406 THU 10:15

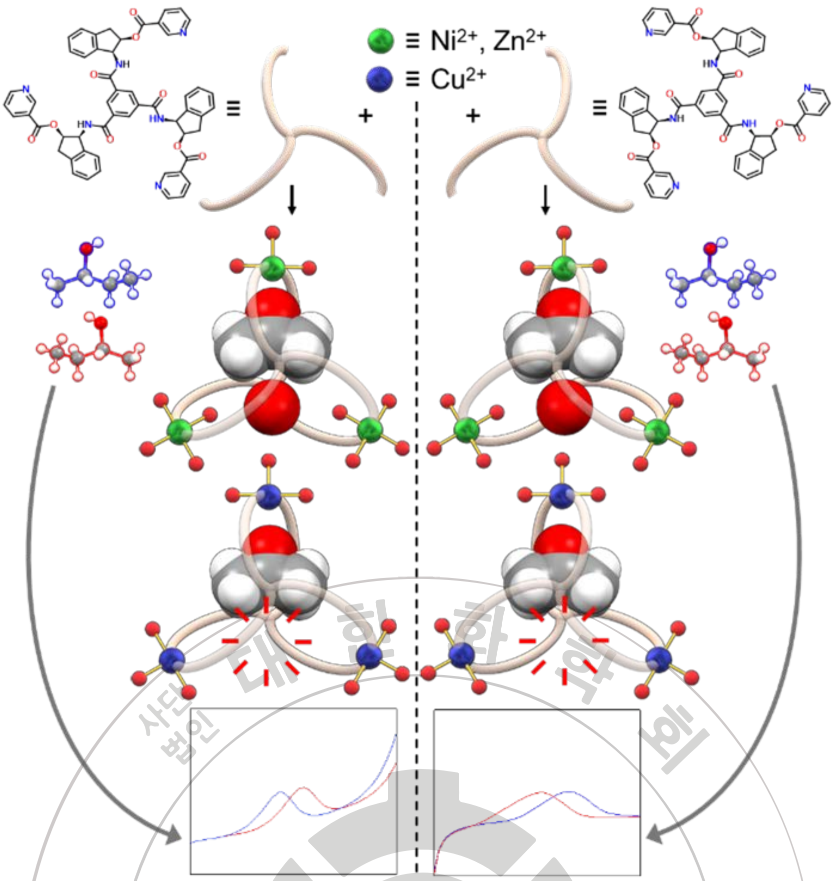
Chair: Jin Yeong Kim (Seoul National University)

Chiral Recognition Using Pairs of Chiral Coordination Cages

Dongwon Kim, Ok-Sang Jung[1], Dohyun Moon[*]

Beam Operation Team, Pohang Accelerator Laboratory, Korea
[1]*Department of Chemistry, Pusan National University, Korea*

Self-assembly of $M(ClO_4)_2$ (M^{2+} = Ni^{2+}, Cu^{2+}, and Zn^{2+}) with (1*S*,1'*S*,1"*S*,2*R*,2'*R*,2"*R*)-(benzenetricarbonyltris(azanediyl))tris(2,3-dihydro-1H-indene-2,1-diyl) trinicotinate (*s*,*r*-L) and the corresponding enantiomer (*r*,*s*-L) as a pair of chiral tridentate donors gives rise to the chiral cage pairs $[M_3$(*s*,*r*- and *r*,*s*-$L)_2](ClO_4)_6$. For the two pairs of $[(Me_2CO)(H_2O)@M_3$(*r*,*s*- and *s*,*r*-$L)_2](ClO_4)_6$ (M^{2+} = Ni^{2+} and Zn^{2+}), the inner cavity is occupied by both an acetone and a single water molecule, whereas for the copper(II) pair of $[Me_2CO@Cu_3$(*r*,*s*- and *s*,*r*-$L)_2](ClO_4)_6$ under the same condition, the cavity is filled by only one acetone molecule. Thus, the encapsulation of guest molecules into the cages during self-assembly shows a significant Jahn-Teller distortion effect. These chiral cages are effective for enantio-recognition of chiral (*S*)-2-butanol and (*R*)-2-butanol via the shifts of the electrochemical oxidation potentials obtained by the electrochemical methods, density functional theory (DFT) calculations, and the chiral 2-butanol adsorption in the single-crystal-to-single-crystal (SCSC) mode.


≡ Ni^{2+}, Zn^{2+}
≡ Cu^{2+}
≡
+
+
≡

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 405+406 THU 10:30

Chair: Jin Yeong Kim (Seoul National University)

Enhancing Stability in Humid Environments for Effective Carbon Dioxide Capture: Hydrophobic Modification of Diamine-Mg_2(dobpdc)

Jong Hyeak Choe, **Chang Seop Hong**[*]

Department of Chemistry, Korea University, Korea

Global warming is accelerating due to the emission of CO_2 into the atmosphere, and it is crucial to remove CO_2 for the survival of mankind. Metal-organic frameworks (MOFs) serve as a promising type of adsorbent, with diamine-appended Mg_2(dobpdc) showing outstanding performance in CO_2 capture. However, the utilization of diamine-appended Mg_2(dobpdc) for practical CO_2 capture is premature due to its low reusability in the presence of water vapor in flue gas. Therefore, to enhance the stability of diamine-Mg_2(dobpdc) under humid conditions, we further modified it by using hydrophobic epoxide and carbonate compounds. Consequently, we obtained surface-modified diamine-Mg_2(dobpdc) with increased hydrophobicity. The resulting adsorbents each exhibited excellent hydrophobicity and maintained structural stability and adsorption performance even under humid conditions. Particularly, these materials retained high CO_2 capacities even after adsorption-desorption cycles in environments with 5% and 10% water vapor, respectively. Further details can be found in the presentation.J. H. Choe et. al. J. Am. Chem. Soc. 2022, 144, 10309.J. H. Choe et. al. J. Am. Chem. Soc. 2024, 146, 646-659.

Oral Presentation : **INOR.O-8**
Oral Presentation of Young Scholars in Inorganic Chemistry
Room 405+406 THU 10:45
Chair: Jin Yeong Kim (Seoul National University)

Rational Synthetic Strategy for Multicomponent Porphyrinic Metal-Organic Frameworks Targeting Advanced Functionality

Junghye Lee, HongKyu Lee[1], Jaeheung Cho[2], Hoi Ri Moon[3,*], Hyunchul Oh[*], Wonyoung Choe[4,*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Chemistry, Ulsan National Institute of Science and Technology, Korea*
[2]*Department of Chemistry, UNIST, Korea*
[3]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*
[4]*Department of Chemistry, Ulsan National Institute of Science and Technology, United States*

Metal-Organic Frameworks (MOFs) have emerged as a promising class of crystalline porous materials, garnering significant attention for their potential in diverse fields such as heterogeneous catalysis, gas storage/separation, and energy transfer due to their high surface area, porosity, and highly tunable structures based on reticular chemistry. Two pivotal approaches have been developed to design advanced MOFs with targeted applications. They are: 1) to design the organic linker with strategic placement of functional groups; and 2) to use multiple organic/or inorganic building blocks for MOF construction. Research on multicomponent MOFs expands the structural complexity and enriches sophisticated applications. Notably, the merged-net approach enables the systematic structural design methodologies of multicomponent MOFs and led to the fascinating development of structural complexity and regulation. This approach is still in its infancy, it is important to discover numerous possibilities for the enrichment of the reticular chemistry. This talk focuses on the strategic structural design of advanced MOFs and their functional applications, particularly emphasizing the rational design of MOF structures based on porphyrin and related linkers, thus offering fresh insights into advanced functional applications such as water sorption, gas sorption and catalysis.

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Oral Presentation : **PHYS1.O-1**

Oral Presentation for Initiative and Next-Generation Physical Chemists I

Room 401+402 THU 09:00

Chair: JaeHong Park (Ewha Womans University)

Modulating light scattering and absorption for active structural colors

Jerome Hyun

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

Structural colors refer to colors arising from the scattering and interference of light by judiciously designed nanostructures. To be viable candidates for display or smart colorimetric sensing applications, their responses must be dynamic. To this end, our lab has worked on designs that can be tuned by a suite of external stimuli including electricity, humidity, and chemical vapor. Unlike plasmonic designs that require the excitation of surface plasmons, our approach mainly relies on photonic responses such as Mie resonances and dielectric waveguide-array modes which free our system from ohmic damping and the interdependence between wavelength and intensity. We also extend our approach to the microwave regime where unprecedentedly thin electromagnetic wave absorbers are realized.

Oral Presentation : **PHYS1.O-2**

Oral Presentation for Initiative and Next-Generation Physical Chemists I

Room 401+402 THU 09:24

Chair: JaeHong Park (Ewha Womans University)

Molecular dynamics simulation study of the defense mechanism against doxorubicin permeation in cancer cell membranes

Namho Kim, Hyonseok Hwang*

Department of Chemistry, Kangwon National University, Korea

The multi-drug resistance (MDR) in cancer is frequently accompanied by alteration of membrane lipid composition that influences drug membrane transport. The doxorubicin (DOX) is an anti-cancer drug used to treat a wide range of cancers, but long-term medication leads to drug resistance with increase in membrane cholesterol (CHOL) ratio. In this research, we investigated the membrane transport mechanism of DOX using molecular dynamics (MD) simulations to elucidate the effect of molecular protonation state and membrane lipid composition on this process. To solve this out, we constructed the membrane models having different ratios of CHOL with two ionized state of drug (neutralized DOX0 and protonated DOXP) considering acidic tumor microenvironment. The free energy profiles revealed that higher CHOL ratio in lipid bilayer resulted in the greater the energy barriers in both forms, but more rapid and higher energy barrier is observed in the case of DOXP. Furthermore, DOX0 induced mild membrane deformation in the CHOL free system enabling water penetration into lipid bilayer, but the water penetration was significantly inhibited in the presence of CHOL. On the other hands, severe membrane disruptions were observed in DOXP systems regardless of the presence of CHOL. These findings suggest that DOX exhibits different permeation mechanisms depending on protonation state: “solubility diffusion” for DOX0 and “ion-induced defect” for DOXP. The calculated effective permeability coefficients of model systems indicate a strong inhibitory effect of membrane CHOL on DOX permeation, which is further enhanced by drug protonation. Taken these together, our research suggests that cancer cells develop drug resistance by elevating membrane CHOL content and acidifying the extracellular environment.

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Oral Presentation : **PHYS1.O-3**
Oral Presentation for Initiative and Next-Generation Physical Chemists I
Room 401+402 THU 09:36
Chair: JaeHong Park (Ewha Womans University)

A Simulation Study on the Effects of Curvature on Unilamellar Vesicle of DPPC lipids and Cholesterol

Jaeheon Yang, Bong June Sung[1,*]

Department of chemistry, Sogang University, Korea
[1]*Department of Chemistry, Sogang University, Korea*

The curvature is one of the important intrinsic properties of biological systems but has been often ignored in many studies. The curvature is even a dynamic property that can change during various biological processes like cell fusion and budding. And the value of the curvature ranges broadly and can be very large like in exosomes and small unilamellar vesicles. The large curvature leads to the asymmetry within membranes, thus influencing the molecular distribution and diffusion of membrane components. But the effects of curvature remain unclear. In this study, we perform extensive molecular dynamics simulations up to 5 μs of (1) unilamellar vesicles of DPPC lipids and cholesterol with curvature inversely proportional to their radius and (2) flat membranes with no curvature, both with varying cholesterol mole fractions. We find that the condensing effect of cholesterol, i.e. the slowing down of diffusion of membrane components, becomes relatively weak in the convex outer leaflet of lipid vesicles. The curvature also makes the orientation of the lipid tail more disordered. Most interestingly, due to the curvature, the inter-leaflet diffusion (or the flip-flop) of cholesterol slows down significantly by up to an order of magnitude.

Oral Presentation : **PHYS1.O-4**

Oral Presentation for Initiative and Next-Generation Physical Chemists I

Room 401+402 THU 09:48

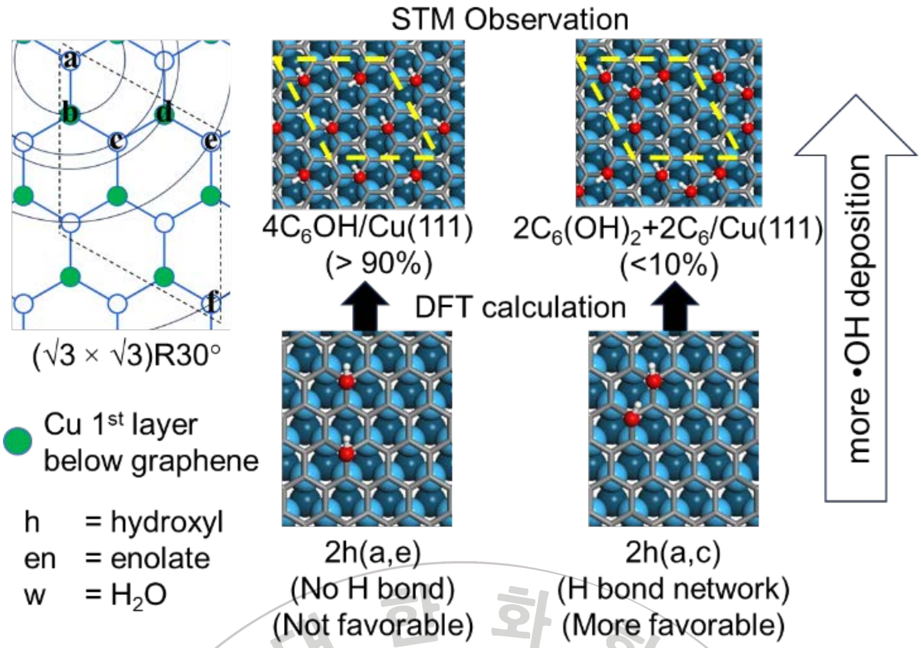
Chair: JaeHong Park (Ewha Womans University)

Enolate-mediated formation of two-dimensional (√3 × √3)R30°-C_6OH graphenol beyond hydrogen bonding network

<u>Rizky Hadiputra</u>, Jaehoon Jung*

Department of Chemistry, University of Ulsan, Korea

We unravel the formation mechanism of highly ordered graphenol (C_6OH) on Cu(111), which was previously reported by scanning tunneling microscopy (STM). The experimentally observed superstructure cannot be simply explained, despite the stabilization of hydroxyl groups via hydrogen bonding. Here, our computational investigation based on density functional theory (DFT) suggests that formation of enolate is crucial to understanding unusual superstructure formation, i.e., graphenol (C_6OH), which is closely related to the interfacial interaction between graphenol and Cu(111). The analysis on potential energy surfaces of hydroxyl adsorption as well as geometric and electronic properties of the formation mechanism of graphenol on Cu(111) provides the crucial details to unveil the role of enolate in the experimental growth mechanism of graphenol superstructure observed by STM. This study extends our understanding by providing an in-depth insight into uniform functionalization of graphene sheet to control its chemical and physical properties.


STM Observation
a
b
c
d
e
f
(√3 × √3)R30°
$4C_6OH/Cu(111)$
(> 90%)
$2C_6(OH)_2+2C_6/Cu(111)$
(<10%)
DFT calculation
more •OH deposition
Cu 1st layer below graphene
h = hydroxyl
en = enolate
w = H_2O
2h(a,e)
(No H bond)
(Not favorable)
2h(a,c)
(H bond network)
(More favorable)

Oral Presentation : **PHYS1.O-5**
Oral Presentation for Initiative and Next-Generation Physical Chemists I
Room 401+402 THU 10:00
Chair: JaeHong Park (Ewha Womans University)

fs-Imaging of Charge Carrier Transport in Perovskite Thin Films

Jooyoung Sung

Department of Physics and Chemistry, DGIST, Korea

Carrier transport dynamics in solid-state semiconductors play a pivotal role in achieving high device performance. A deep understanding of how charge carriers transport in bulk/thin semiconductors will shed light on developing next-generation semiconductors. However, the observation of true charge carrier transport has hardly been reported due to limitations in time- and space-resolved techniques. In brief, space-resolved spectroscopy techniques, such as TEM, SEM, and various types of optical microscopy, offer excellent spatial resolving power but with poor time resolution. On the other hand, time-resolved spectroscopy techniques, such as TAS, TRPL, etc., have good time-resolving capabilities but lack good spatial resolution. This necessitates a new type of integrated time- and space-resolved technique. In this talk, I will first introduce a new type of time- and space-resolved spectroscopy technique called transient absorption microscopy (TAM), which offers dual capabilities: femtosecond time resolution and nanometer-scale spatial resolution. I will then discuss the application of TAM to perovskite thin films, which exhibit ballistic transport of non-equilibrium charge carriers with transport lengths of up to 150 nm. I will further explore how the non-equilibrium charge carrier dynamics are influenced by the nanoscale chemical heterogeneity, as revealed by fs-microscopic measurements on alloyed perovskite thin films. Finally, I will discuss very recent observations on transient circular dichorismic property of formaidium lead iodide based perovskite thin films.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Oral Presentation : **PHYS1.O-6**

Oral Presentation for Initiative and Next-Generation Physical Chemists I

Room 401+402 THU 10:24

Chair: JaeHong Park (Ewha Womans University)

Enantioselective Detection of Monosaccharides by Surface-Enhanced Raman Spectroscopy

Daedu Lee, Yoonsoo Pang*

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

Chiral detection has been considered crucial in the fields of biomedicine, pharmaceutics, *etc.* since many physiological processes in living systems involve the intermolecular interactions between the molecules of specific chirality. Circular dichroism (CD) has been commonly used in chiral detection, but the applications are rather limited by high sample concentrations and insufficient molecular-level information. Surface-enhanced Raman spectroscopy (SERS) has emerged as one of the alternatives to CD due to its extremely high sensitivity and molecular-specific vibrational information. The chirality of target molecules can be identified from the SERS spectral changes of reporter molecules by the chiral-selective molecular interactions. However, how chirality controls the surface adsorption and molecular orientation of the target and reporter molecules at the molecular level, is not yet fully understood.In this study, SERS-based chiral sensing of glucose (Glu) and fructose (Fru) was investigated, where a chiral aromatic amino acid, phenylalanine (Phe) was adopted as a reporter molecule. The Phe SERS spectra show spectral changes only when the Glu or Fru of the same chirality as Phe was added. The vibrational modes, including $\delta(\mathrm{COO}^-)$, $\nu_s(\mathrm{COO}^-)$, and ring modes, are strongly dependent on the surface adsorption geometry of Phe. As the surface adsorption of Phe via carboxylate changes from the bidentate to monodentate interactions, the relative intensities of these marker bands show concentration-dependent changes. Quantitative detections of Glu or Fru in the wide concentration range of 2×10^{-5} ~ 2×10^{-9} M were obtained in a good linear correlation with the relative intensity changes of Phe-SERS.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Oral Presentation : **PHYS1.O-7**

Oral Presentation for Initiative and Next-Generation Physical Chemists I

Room 401+402 THU 10:36

Chair: JaeHong Park (Ewha Womans University)

Correlating the Crystallographic and Photophysical Attributes: Cubic-Shaped ZnSeTe QDs with Bright and Narrow-Band Blue Emission

Yu Jin Lee, Dongho Kim[*]

Department of Chemistry, Yonsei University, Korea

The escalating demand for the commercialization of self-luminescing quantum dots (QD) light-emitting diodes (LEDs) has fueled extensive research into the development of environmentally friendly and efficient QD materials. This study adopts a combination of crystallographic and spectroscopic approaches to unravel the intricate relationship between the cubic particle shape and the heightened emitting properties of blue-emitting ZnSeTe QDs. The introduction of hydrofluoric acid (HF) additive yields a remarkable quantum yield (QY) of 97% with an ultranarrow peak width of 14 nm. The induced morphology change stems from a selective exposure of stabilized (100) facets, leading to reduced lattice disorder and defect formation. Thorough time-resolved spectroscopic studies are employed to extend the lattice structure investigation and comprehend the role of HF treatment in reducing defect density and tailoring the optical properties of ZnSeTe QDs. This provides invaluable insights into the growth mechanism and factors influencing QD photoluminescence efficiency. The elucidation of the photoluminescence mechanism concerning lattice structure positions ZnSeTe QDs as promising contenders for blue-emitting QD-LED materials. The successful optimization of photoluminescence properties through hydrofluoric acid (HF) treatment, coupled with the profound insights gained into the photoluminescence mechanisms, offers crucial guidance for advancing the development and commercialization of efficient and eco-friendly quantum dot materials. These advancements hold the potential to revolutionize next-generation self-luminescent displays.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Oral Presentation : **PHYS1.O-8**
Oral Presentation for Initiative and Next-Generation Physical Chemists I
Room 401+402 THU 10:48
Chair: JaeHong Park (Ewha Womans University)

Computational Analysis of Brook Rearrangement Mechanism

Ka young Cho, Jaehong Park*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The Brook rearrangement is one of the most important reactions in synthetic chemistry as it allows for the synthesis of benzene. However, in specific Brook rearrangements, it is difficult to determine the direction in which the reaction proceeds. The mechanism I will introduce in this presentation has two possibility: 1,3 shift and 1,5 shift. However, as is well known, it is difficult to experimentally determine the mechanism path of these organic reactions. Therefore, I tried to reveal the meachanism through computational chemistry. Density Functional Theory was used, and geometry optimization and single-point energy calculation were conducted.

Oral Presentation : **PHYS2.O-1**

Oral Presentation for Initiative and Next-Generation Physical Chemists II

Room 401+402 FRI 09:00

Chair: Taeyeon Kim (Sungkyunkwan University)

Research on Degradation and Phase transition of Semiconducting Nanomaterials

Hanleem Lee

Myungji University, Korea

Semiconducting nanomaterials, such as quantum dots, nanorods, and thin films, play critical roles in a wide range of applications, including electronics, photonics, and optoelectronics. However, these materials can degrade over time due to environmental factors such as exposure to light, heat, moisture, and chemical contaminants. For commercialization, investigating the degradation pathways and phase transitions of semiconducting nanomaterials is important to develop strategies for enhancing their stability and reliability. Recently, researchers have been exploring methods for mitigating degradation effects and stabilizing semiconducting nanomaterials through surface passivation, encapsulation, and interface engineering. In this study, we investigate the degradation mechanism of perovskite quantum dots (QDs) and find that the kinetics of surface ligands [1], phase transition [2], and cation migration [3] play crucial roles in perovskite QD degradation. Through in-situ transmission electron microscopy studies, we observe a high number of defects in the deep core sites that can propagate to the surface during cation migration, leading to structural degradation originating from surface defects. To mitigate the degradation of perovskite QDs, ultrathin shell coatings (i.e., SiO2 and MoWSe2) [4] have been proposed. The core-shell structure effectively passivates surface defects and prevents defect propagation. Especially, amorphous MoWSe2 effectively passivates core perovskite materials through van der Waals interactions, resulting in high-temperature resistance (up to ~300°C) and excellent electrical properties (1 mA in a 0.5M Na2SO4 aqueous solution). The remarkable control over the perovskite QDs ink allows us to fabricate micro-sized patterned perovskite quantum dot LEDs with high luminescence using both red and green perovskite QDs. [1]

Oral Presentation : **PHYS2.O-2**

Oral Presentation for Initiative and Next-Generation Physical Chemists II

Room 401+402 FRI 09:24

Chair: Taeyeon Kim (Sungkyunkwan University)

Large-Scale Photoelectrochemical Simulations in Solutions Using Many-Body Perturbation Theory

Se-Jun Kim, **Hyungjun Kim***

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

The intricate chemical phenomena occurring in the real world are often influenced by external factors such as light, electricity, or solvent environments. To comprehensively understand this chemical complexity, advanced simulation methods become indispensable. In this study, we introduce a novel methodology based on many-body perturbation theory. Specifically, we address the challenge of understanding fundamental chemistry at the solid-liquid interface, wherein multiple factors is needed to be considered simultaneously. Our proposed method accurately reproduces critical band edge positions, such as the valence band maximum (VBM) or conduction band minimum (CBM) in water, aligning closely with experimental measurements. Additionally, our method demonstrates excellent agreement with optical experiments in predicting optical spectra and excitonic behavior. Finally, we outline future directions for our methodology, emphasizing its potential for large-scale simulations of (photo)(electro)chemical systems. We believe that our approach represents a superior method to unravel the enigmatic chemistry at the solid-liquid interface, paving the way for significant advancements in the field.

133rd General Meeting of the Korean Chemical Society
April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Oral Presentation : **PHYS2.O-3**
Oral Presentation for Initiative and Next-Generation Physical Chemists II
Room 401+402 FRI 09:36
Chair: Taeyeon Kim (Sungkyunkwan University)

Dynamical phase transitions of spin-lattice models using double-bias trajectory ensemble methodology

Jay-Hak Lee, YounJoon Jung*

Department of Chemistry, Seoul National University, Korea

Systems far-from-equilibrium have various properties that are different from systems in equilibrium. However, from the perspective of equilibrium statistical mechanics, these states are considered rare events with higher free energy compared to the equilibrium state, making them challenging to study. Recently, a trajectory ensemble methodology has emerged that can sample and study systems in a non-equilibrium state using large-deviation theory. From this methodology, dynamical phase transition which is analogous to equilibrium thermodynamics emerged, and various non-equilibrium states such as the glass phase could be explained. In this work, two-dimensional phase diagrams of various lattice models are obtained by applying s,g-ensemble that biases both the dynamical activity and trajectory energy of the system. First, in the one-dimensional Ising model, dynamical free energy is obtained analytically and phase transitions that did not exist in the equilibrium state are observed. Next, the correlation between dynamical activity and trajectory energy is observed in the kinetically constrained model which simulates the glass phase, and finite size scaling of the dynamical phase transition is performed. With this approach, we can theoretically approach various unique properties that appear in non-equilibrium.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Oral Presentation : **PHYS2.O-4**

Oral Presentation for Initiative and Next-Generation Physical Chemists II

Room 401+402 FRI 09:48

Chair: Taeyeon Kim (Sungkyunkwan University)

Quantum Chemical Studies on the Rates and Stereoselectivities in Energy Transfer Photocatalysis

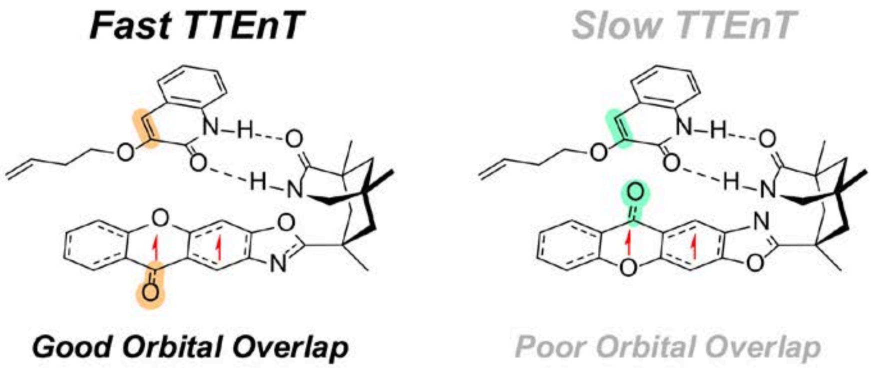
Jiyong Park*, **Mu-Hyun Baik**[1]

Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea

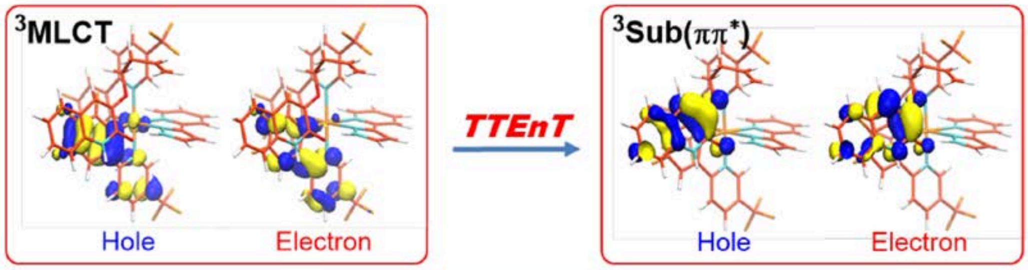
[1]*Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Organic and organometallic triplet sensitizers have emerged as potent photocatalysts, that can activate substrates into triplet excited-state intermediates. These sensitizers, upon irradiation, rapidly access triplet excited-state manifolds and transfer the excited-state character to the substrates via the triplet-triplet energy transfer (TTEnT) known as the Dexter energy transfer. Despite its potential, the mechanistic details of the TTEnT remain largely unexplored, impeding the rational design of stereoselective photocatalytic transformations based on TTEnT. Herein, we employ quantum chemical methods to characterize the excited state electronic structures of the encounter complexes comprising the sensitizer and substrates. Marcus theory of electron transfer in combination with the theory of diabatic electronic coupling was used to compute the rates of TTEnT. We applied the theoretical framework on the intramolecular [2+2] cycloadditions of quinolones using chiral organic and organometallic triplet sensitizers developed by the Yoon and Bach groups. Our findings suggest that the TTEnT is the rate-determining step of the photocatalytic [2+2] cycloadditions. Additionally, we explore the contrathermodynamic isomerization of E-alkenes to Z-counterparts using thioxanthone as a triplet sensitizer. Our quantum chemical mechanistic study underscores the significance of encounter complexation, leading to differences in the rates of TTEnT, which accounts for the observed stereoselectivity in the photochemical transformations. Our computational analysis provides detailed mechanistic understandings of the emerging class of catalytic transformations that will aid the further development of novel photocatalytic transformations.

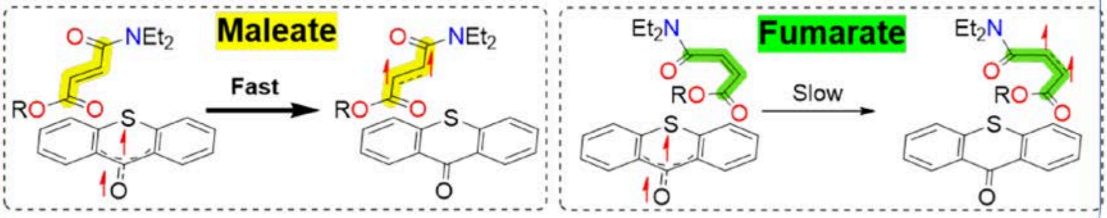
(a) *Mechanism of substrate activation in the photocatalytic [2+2] cycloaddition*



(b) *Role of H-bonding Mediated Complexation in the photocatalytic [2+2] cycloadditions*



(c) *Contrathermodynamic [E]/[Z] Isomerization of alkenes using Thioxanthone*



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Oral Presentation : **PHYS2.O-5**
Oral Presentation for Initiative and Next-Generation Physical Chemists II
Room 401+402 FRI 10:06
Chair: Taeyeon Kim (Sungkyunkwan University)

Active Site Determination in Embedding Calculations: A Density Sensitivity and Orbital Localization Approach

Soohyeon Lee, Youngsam Kim, Eunji Sim[*]

Department of Chemistry, Yonsei University, Korea

Density functional theory (DFT) is a popular method for electronic structure calculations due to its efficiency, but its moderate accuracy may require the use of more computationally expensive methods for accurate results in certain systems. For these systems, embedding methods can be used to achieve both accuracy and low cost. In the embedding method, active sites are defined as important areas of the system and calculated using high-level methods. This reduces the computational cost while maintaining reliable accuracy. Since active sites have a greater influence on chemical properties such as energy, it is important to determine the correct active sites. However, it is not always straightforward to know which area has how much influence. While chemical intuition may be useful in some systems, it may not be applicable in others. In this study, we present an automated approach to determine active sites based on density sensitivity and orbital localization. The density sensitivity is used as an indicator of where chemical properties have more influence and is calculated before embedding using low-level methods. We have developed a method for calculating the density sensitivity of each area of the system and selecting orbitals based on their degree of localization. Our results demonstrate the reliability of this method.

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Oral Presentation : **PHYS2.O-6**
Oral Presentation for Initiative and Next-Generation Physical Chemists II
Room 401+402 FRI 10:18
Chair: Taeyeon Kim (Sungkyunkwan University)

pyMCD: A Python package for an efficient and reliable transition search via the Multicoordinate Driven (MCD) method

Kyunghoon Lee, Woo youn Kim[1,*]

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

The identification of activation barriers is the key information for the elucidation of chemical reactions. The barrier information is only accessible through the transition state (TS) information. While a number of transition state search methods have been developed for the last decades, we focused on the multicoordinate driven (MCD) method for an efficient TS search. The method is particularly useful because of its simple input preparation and high reliability with reasonable computational cost. It searches TS by generating a reaction path by scanning multiple active coordinates until it reaches at the products, starting from the reactants geometry. Despite its high practicality, however, the source code is not publicly available. Herein, we have developed a Python package called pyMCD that searches for TSs using the MCD method, and introduce its practicalness by appplying it to several different types of chemical reactions. We have also implemented a slightly revised version of the original MCD method proposed by Berente and coworkers, where the revised method has much higher computational efficiency while minimizing the loss of accuracy. The package is extremely user-friendly and requires minimal effort from users for input preparation. We believe that our newly developed package can benefit computational chemists in their search for transition states of their own reactions of interest.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Oral Presentation : **PHYS2.O-7**

Oral Presentation for Initiative and Next-Generation Physical Chemists II

Room 401+402 FRI 10:30

Chair: Taeyeon Kim (Sungkyunkwan University)

Luminescent properties of organic neutral radical emitters

Eunkyung Cho

Division of Energy Technology, DGIST, Korea

Neutral donor−acceptor (D−A•) organic radicals have recently attracted a great deal of attention as promising luminescent materials since both the first excited electronic state and the ground state are spin doublets, which results in spin-allowed radiative transitions. We performed long range-corrected density functional theory calculations and theoretical modeling to evaluate how chemical structure of a series of D-A• radicals affects the electronic structures and radiative and non-radiative decay rates. Our calculations show that hybridization between the charge transfer (CT) and ground states of the radicals plays a dominant role in the radiative decay rates, while hybridization between the CT state and the lowest local excitation (LE) state on the TTM radical core has a significant contribution to the non-radiative rates for some radicals. In order to understand the luminescent properties of D−A• radicals, thus, it is important to properly consider the electronic hybridization of the CT states with both the ground and the LE states.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Oral Presentation : **PHYS2.O-8**

Oral Presentation for Initiative and Next-Generation Physical Chemists II

Room 401+402 FRI 10:48

Chair: Taeyeon Kim (Sungkyunkwan University)

Study on Photochromic switching Diarylethene Dopant Design Principle for Extending the Linear Dynamic Range of Organic Photodetector Using Quantum Calculation and Machine Learning

Changwon Choi, Yun Hee Jang[1,*]

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

[1]*Department of Energy Science and Engineering, DGIST, Korea*

Organic photodiodes (OPDs) exhibit several unique advantages over inorganic photodiodes, including smaller diode thickness, color selectivity, and low-temperature solution processablility. However, when the incident light becomes stronger, it saturates relatively early with the photocurrent, making it impossible to detect the object. To solve this, n-type photochromic diarylethene (DAE) dopants are introduced. In dark, the open form of DAE has a Lowest unoccupied molecular orbital (LUMO) similar to organic polymer. It operates as a normal OPD. External holes are not injecting due to the energy barrier between the organic polymer and cathode. As the light becomes stronger, DAE changes to a closed form through photocyclization reaction and LUMO decreases. Electrons are trapped in this lowered LUMO, and the electric field generated by the trapped electrons causes band bending of the organic polymer, allowing additional holes to be injected from the cathode. It operates as an photomultiplication type OPD and the external quantum efficiency exceeds 100%. In order for the photoswitching DAE to function properly, several conditions are required. We are trying to design a DAE molecular structure that meets these conditions. Initially, Highest occupied molecular orbital (HOMO), LUMO, and bandgap in open/closed form for 133 structures were obtained using density functional theory (DFT) and time-dependent DFT. Define dopant requirements according to the type of OPD and select appropriate dopants. Afterwards, this data set are used to infer data about uncalculated candidates through machine learning.

We were able to obtain an additional suitable DAE structure, and by extending the general structure, we propose DAE design principles according to different functional groups.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:00

Chair: Yeonho Kim (Konkuk University)

Simultaneous analysis of 29 banned Illegal dyes in Tattoo ink by Liquid chromatography-Electrospray ionization- tandem mass spectrometry(LC-ESI-MS/MS)

Minkyu Lee[*], **Sangwon Cha**[1,*]

chemistry department / analytical chemistry and mass spectrometry, Dongguk University, Korea

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

In tattooing, coloring agents are injected through microscopic holes in the epidermal layer of the skin and remain in the skin for a long period of time, so it is very important that the dye for tattoo does not contain carcinogenic or allergenic dyes. However, there are no established analytical methods for the 35 tattoo dyes that are legally banned in South Korea. In addition, illegal dyes are divided into various classes according to their structural properties, acidic, basic, disperse, solvent, and pigment classes. Since each class has different physico-chemical properties, simultaneous analysis of all classes of illegal dyes is challenging. In this study, we developed an analysis method for the simultaneous qualitative and quantitative analysis of 29 dyes out of 35 illegal dyes, using liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS). The sample preparation procedure was optimized to increase the recovery rate in the simultaneous analysis of four classes of dyes. The analysis results by the developed method showed good analytical performances, including linearity, sensitivity, accuracy, and precision. These dyes also could be used in cosmetics, textiles, food, etc. due to their cost-effectiveness and intense colors. Therefore, this platform is expected to contribute to the improvement of current safety investigation and monitoring services by enabling simultaneous quantitative analysis of illegal dyes used in products for various purposes, not limited to tattoo inks.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:06

Chair: Yeonho Kim (Konkuk University)

Quantitative Determination of Aromatic Amines Released from Azo Dyes in Tattoo Ink by Gas Chromatography-Electron Ionization-Mass spectrometry(GC-EI-MS) and tandem mass spectrometry(GC-EI-MS/MS)

Hyebeen Kim[*], **Sangwon Cha**[1,*]

Dongguk University, Korea

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

Azo dyes are compounds characterized by their vivid colors and provide excellent coloring properties. They are important and widely used as coloring agents in a variety of industries. The risk in the use of azo dyes arises mainly from the breakdown products that can be created in vivo by reductive cleavage of the azo group into aromatic amines. For this reason, several aromatic amines are classified as carcinogenic, and quantitative analysis of them in various household chemicals is essential. In this study, effective methods for determining hazardous aromatic amine products of azo dyes in tattoo ink products were developed by using gas chromatography-electron ionization-mass spectrometry (GC–EI-MS) and GC-EI-tandem MS (GC-EI-MS/MS). For the identification of the analytes one precursor ion and two daughter ions (multireaction monitoring, MRM) were selected and the GC-MS/MS parameters were optimized to achieve high sensitivity and selectivity. The developed method with GC-MS/MS showed superior analytical performances over conventional methods listed in international organization for standardization (ISO). Therefore, we expect that the method developed in this study can replace the current ISO methods and can be applied to a wide range of products containing dyes, not just tattoo inks.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:12

Chair: Yeonho Kim (Konkuk University)

Chemical Fingerprinting Analysis of Pen Ink and Dyes by Matrix-assisted Laser Desorption Ionization and Capillary Electrophoresis

Jaeyoung Heo[*], **Sangwon Cha**[1,*]

Dongguk university, Korea

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

There are many different substances present in commonly used pens. Even pens of the same color have very different types of dyes and polymers depending on the make and model, and the ingredients are not disclosed in detail due to patents. One of the key issues in forensic document analysis is determining which pen was used for two different documents or letters written with the same color pen and in the same handwriting. Therefore, to solve this problem, it is necessary to establish a database that can identify the type of pen based on the chemical fingerprint of the pen ink. In order to achieve this, we utilized matrix-assisted laser desorption ionization mass spectrometry (MALDI MS) and capillary electrophoresis (CE) as chemical fingerprinting analysis plaforms for pens. First, we optimized MALDI experimental conditions for MALDI MS including choices of matrix and extraction solvents mass spectra. Then, we collected MALDI mass spectra of pen dye standards and various pens to establish a database. For fingerprinting analysis for pens containing anionic dyes that are relatively difficult to analyze with MALDI MS, we performed additional chemical fingerprinting analysis with CE. We believe that the binary and highly orthogonal data obtained through MALDI MS and CE can contribute to improving the reliability of pen identification.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:18

Chair: Yeonho Kim (Konkuk University)

Improved electrochemical sensor performance of Graphene incorporated Vanadium-Silver oxide nanocomposite modified electrode for selective determination of chlorpyrifos pesticides

Gunasekaran Manibalan, Ji Won Ha[*]

Department of Chemistry, University of Ulsan, Korea

This research work aims to develop a low cost electrocatalyst with high performance electrochemical sensor applications for graphene incorporated vanadium-silver metal-oxide nanocomposite glassy carbon modified electrode. Herein, the heterostructure Graphene/V2O5-Ag2O nanocomposite was synthesized by facile hydrothermal route. The structural and morphological characteristics of nanocomposite were inspected using X-ray diffraction (XRD), scanning electron microscopy (SEM), and high-resolution transmission electron microscopy (HR-TEM) analyses. Further, the electrocatalytic activity of Graphene/V2O5-Ag2O nanocomposite modified electrode for the selective detection of chlorpyrifos organophosphate pesticide was investigated. The electrochemical sensing capability of synthesized electrocatalyst was studied using different electroanalytical techniques such as cyclic voltammetry and cathodic stripping square wave voltammetry analyses. The concentration dependent CV analysis of modified electrode implies a good linear response with excellent sensitivity in the concentration range from 100 to 1000 µM. From the cathodic stripping square wave voltammetry studies, the sensitivity and selectivity of the modified electrode was evaluated. The sensitivity and limit of detection (LOD) of the modified electrode exhibits the 0.480 µA µM-1 with co-relation coefficient of R2= 0.998 and 0.045 µM, respectively. Also, the selectivity of the modified electrode was demonstrated in the presence of other interfering molecules that were studied for selective determination of chlorpyrifos organophosphate analyte. Similarly, the better performance of reproducibility and stability of the modified electrode. The proposed sensor revealed the successfully established a low-cost, and improved electrocatalytic activity of

Graphene/V2O5-Ag2O electrocatalyst towards the detection of chlorpyrifos organophosphate pesticide for environmental applications.

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April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:24

Chair: Yeonho Kim (Konkuk University)

CRISPR/Cas12a-assisted Au Nanowire SERS Sensor for ATP Detection

Toeun Kim, Hongki Kim*

Kongju National University, Korea

The clustered regularly interspaced short palindromic repeats (CRISPR)-Cas12a system has gained significant attention in molecular diagnostics for its simplicity, sensitivity, specificity, and wide range of applications. The current CRISPR/Cas12a sensing system has been adopted for detecting not only nucleic acids but also non-nucleic acids, leveraging its collateral cleavage capability. In this study, we report the CRISPR/Cas12a-based Au nanowire surface-enhanced Raman scattering (SERS) sensor for detecting adenosine triphosphate (ATP). In the presence of ATP, the locked activators composed of ATP aptamer and DNA activator induce the release of the DNA activator. This released DNA activator is specifically recognized by Cas12a/crRNA complex and activates cleavage of Cy5-labeled single-stranded DNA attached to the Au nanowire, resulting in reduced SERS intensity. With this approach, we effectively convert the recognition of ATP into a detectable SERS signal. This research will broaden the scope of applications for the CRISPR-Cas detection system and offer a practical method for the analysis of non-nucleic acid targets.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:30

Chair: Yeonho Kim (Konkuk University)

Sex-specific reproductive dysfunction in zebrafish: Estrogenic and anti-androgenic effects of 4-tert-octylphenol

Jangjae Lee, Yunji Kim, Sung-Hee Cho*, Hugh I. Kim[1]

Center for Chemical Analysis, Korea Research Institute of Chemical Technology, Korea

[1]Department of Chemistry, Korea University, Korea

Alkylphenols, such as nonylphenol and 4-tert-octylphenol (OP), are estrogenic chemicals generated through the breakdown of alkylphenol ethoxylates, posing risks to aquatic life and higher organisms. In this study, we examined OP's toxic influence on the reproductive hormones of both female and male zebrafish. For 21 days, the zebrafish were subjected to four OP concentrations (0, 20, 100, and 500 ng/mL), selected based on the minimum concentration (EC10 = 0.48 ng/mL) affecting zebrafish embryos. OP exposure led to a significant rise in liver vitellogenin mRNA levels and 17β-estradiol production in both genders. Conversely, OP's anti-androgenic impact was observed as a decrease in gonadal androgen receptor (AR) mRNA levels and a reduction in endogenous androgens (testosterone and 11-ketotestosterone) in males. Notably, cortisol and thyroid hormone concentrations increased with OP dosage in both sexes, influencing the regulation of gonadal steroids. Our data indicate that extended OP exposure results in persistent reproductive issues in adult zebrafish, largely due to the complex interactions between hormone levels and associated gene expressions. By conducting comprehensive biological response assessments in adult zebrafish, our findings offer essential insights into OP's reproductive toxicology, supporting further studies in aquatic environments.

Oral Presentation : **ANAL1.O-7**
Oral Presentation of Young Analytical Chemists I
Room 103+104 THU 09:36
Chair: Yeonho Kim (Konkuk University)

A method for quantification of formaldehyde in phenolic resin using 13C NMR spectroscopy

Jeaheung Park, Daye Kwon, Jungmin Oh*

Analysis & Evaluation Team 1, KOLON INDUSTRIES, Korea

Unreacted formaldehyde remains in the phenol resin after completion of manufacturing. Since formaldehyde is a carcinogenic and hazardous substance, the amount of exposure to the human body must be minimized, so when manufacturing phenolic resin, a scavenger is added in the final process to reduce its content. The mainly used scavenger is urea, which reacts with formaldehyde to form urea-formaldehyde resin. Generally, formaldehyde is derivatized using DNPH (2,4 Dinitrophenylhydrazine) and analyzed by HPLC. Using this method has the advantage of being able to detect formaldehyde with a general ultraviolet detector, and paraformaldehyde in the form of self-polymerization by reacting with water can also be derivatized and analyzed by including it in the formaldehyde content. However, in the presence of urea-formaldehyde polymer, formaldehyde is decomposed and reacts with DNPH, so the residual amount cannot be accurately analyzed after the formaldehyde reduction process, and a value higher than the actual amount is observed. To solve this problem, we developed a method to accurately measure the content of formaldehyde remaining after urea injection using 13C NMR spectroscopy.

Oral Presentation : **ANAL1.O-8**

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:42

Chair: Yeonho Kim (Konkuk University)

Stability and sensitivity enhanced paper-based nonenzymetic label-free SERS biosensor for glucose detection

Rashida Akter, Hongki Kim[1,*]

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Glucose detection has an essential diagnostic importance for diabetes control and monitoring. In this work, we have fabricated a stability and sensitivity enhanced paper based nonenzymatic and label free SERS biosensor for glucose detection. The SERS biosensing platform is fabricated by modifying the cellulose paper (CP) with a naturally derived polymer, chitosan (CS), followed by depositing enormous amount of plasmonic silver nanoparticles (AgMPs) on CP/CS and finally forming a self-assembling monolayer of mercaptophenylboronic acid (MPBA) on CP/CS/AgNPs. The SERS platform is characterized by SEM EDX, and XRD techniques. The glucose detection is achieved by monitoring the intensity of C-S stretching band and 1072 cm^{-1} in MPBA, which is gradually increased with increasing concentration of glucose due to the increased orientation change of MPBA on AgNPs. The results show that the proposed glucose SERS biosensor exhibits high sensitivity with a limit of detection (LOD) of 0.74 mM and linear dynamic range between 1.0 and 7.0 mM. The practical application of this SERS biosensor for the glucose detection in real samples are currently in progress.

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Oral Presentation : **ANAL1.O-9**
Oral Presentation of Young Analytical Chemists I
Room 103+104 THU 09:48
Chair: Yeonho Kim (Konkuk University)

Development of a nucleic acid extraction device based on photothermal magnetic nanoparticles

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Nucleic acid extraction, a pivotal process in molecular biology, finds diverse applications ranging from diagnostic assays to cutting-edge research endeavors. However, conventional extraction methods often encounter challenges such as complexity, time consumption, and limitations in on-site deployment. This study aims to develop a device utilizing plasmonic nanoparticles for streamlined and expeditious nucleic acid extraction. Plasmonic nanoparticles possess the capability to absorb light of specific wavelengths from an external light source, generating heat as a result. Leveraging this property, these nanoparticles can effectively disrupt cell membranes. The silica shell of plasmonic nanoparticles offers heightened stability and a vast surface area, facilitating efficient binding and extraction of nucleic acids. Furthermore, the magnetic properties of the nanoparticle core enable facile separation. This research endeavors to harness these characteristics in designing a straightforward device for nucleic acid extraction and validate its efficacy. Such a device holds promise for on-site nucleic acid extraction applications with substantial potential across various fields including medical diagnostics, environmental monitoring, and biopharmaceutical production.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 09:54

Chair: Yeonho Kim (Konkuk University)

Hyperspectral NIR measurement of dried seaweeds for determination of their protein contents

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Hyperspectral imaging has gained widespread attention across various sectors, including agriculture area, owing to its rapid detection speed and ability to measure large areas. However, a notable limitation arises when dealing with thin samples, as the interaction of NIR radiation with the sample may not be sufficient to produce component-specific spectra with good signal-to-noise ratios. To solve this problem, PTFE was employed as a sample measurement plate, since it is an effective beam-diffusing medium with high reflectance. Therefore, this approach induces a trans-reflectance sample interaction, thereby increasing the number of photons interacting with the sample. To evaluate the usage of this proposed scheme, the NIR measurement of dried seaweeds, thin samples, were performed to determine their protein contents. A total of 51 sheets of dried seaweeds was measured by using both hyperspectral NIR and conventional transmission NIR instrumentations. Among the hyper NIR spectra, the spectra obtained at the well-focused regions were separated by k-nearest neighbor algorithm for subsequent quantitative analysis. Also, the transmission NIR spectra were collected by scanning over a similar area in the sample with a moving stage. Finally, partial least squares (PLS) was executed using both acquired data and errors in the determination of protein contents were compared.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:00

Chair: Yeonho Kim (Konkuk University)

Efficient feature extraction using convolutional autoencoder (CNNAE) for hetero spectral two-trace two-dimensional (2T2D) correlation maps and interpretation using Grad-CAM

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Two-trace two-dimensional (2T2D) correlation analysis, which uses a pair of spectra instead of a series of spectra, has been widely used for various studies in vibrational spectroscopic analysis. It has the advantage of maximizing even minute differences in the spectra. Meanwhile, a 2T2D map data has an excessive number of features, which limits its direct use for discrimination analysis. So, only data of a slice spectrum at v (n×1 features) is typically used for subsequent analysis. However, information from the remained slice spectra, which would be still valuable for a target analysis, will be lost in this case. Additionally, Grad-CAM was used to interpret feature extraction through CNNAE. Grad-CAM enables the identification of the specific features that the convolutional layer deems significant. With the proposed method, the NIR and Raman spectra of red pepper powers were employed for the discrimination of their geographical origins and following results were discussed.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:06

Chair: Yeonho Kim (Konkuk University)

Polyethylene glycol for highly efficient enrichment of exosomes derived from human blood serum

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Exosomes are nanosized extracellular vesicles measuring between 30-120 nm, that originate in the endosomal pathway and play crucial roles in intercellular communication. Recently, the applications of exosomes in disease diagnostics, therapeutics, and drug delivery have gained significant interest. In this study, we present an approach for enriching and isolating serum exosomes using polyethylene glycol (PEG) precipitation technique. To remove cells and other large molecules from the serum, the serum was subjected to low-speed centrifugation at 2,000 × g for 30 min, followed by additional centrifugation at 12,000 × g for 45 min. The resulting solution was filtered to remove cells and cell debris. The filtered serum (500 µL) was mixed with PEG and incubated at 4°C for 30 min, followed by centrifugation at 1,500 × g for 30 min. The resulting pellet was then dissolved in 500 µL PBS solution. This procedure was repeated four times. The results from size exclusion chromatography of the samples without PEG enrichment revealed the presence of two peaks, which are probably both protein and exosomes. The later eluting peak disappeared during PEG enrichment, and the most abundant peak was assumed to be exosomes. These results were further confirmed by western blot and scanning electron microscopy. Utilizing the PEG precipitation technique proves to be highly efficient for enriching exosomes from blood serum, offering a cost-effective and efficient substitute for commercially available products.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:12

Chair: Yeonho Kim (Konkuk University)

SERS-based assay of uropathogen using magnetic beads immobilized with gold nanoparticles

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The current gold standard method for the diagnosis of urinary tract infection (UTI) is urine culture. However, this method takes at least two days to obtain assay results and usually requires additional complicated steps, such as biochemical tests, polymerase chain reaction (PCR), or mass spectrometry to confirm whether the isolated strain is the pathogen of interest. To address these issues, we developed magnetic beads immobilized with gold nanoparticles (MB-AuNPs) as a surface-enhanced Raman scattering (SERS) substrate. The MB-AuNPs offer several advantages, including excellent magnetic properties that simplify the assay procedures and good SERS properties resulting from densely packed AuNPs. By using these MB-AuNPs, we performed a sensitive and rapid SERS-based assay to detect the most common bacterial species causing UTI, E. coli.

Oral Presentation : **ANAL1.O-14**
Oral Presentation of Young Analytical Chemists I
Room 103+104 THU 10:18
Chair: Yeonho Kim (Konkuk University)

Highly sensitive detection of SARS-CoV-2 RNA using CRISPR/Cas13a-mediated SERS-based dual-flow assay strip

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The gold standard method for diagnosing SARS-CoV-2 target gene is RT-PCR. However, amplifying the target gene requires a reverse-transcription and thermocycling process, taking approximately 3-4 hours. Due to the rapid spread of the virus, the lateral flow assay (LFA) strip is also employed as a diagnostic method. This approach is quick and simple but exhibits a high false-negative rate due to limitations of detection sensitivity. The trans-cleavage activity of the CRISPR/Cas system has recently demonstrated excellent potential for sensitive and rapid detection of the target gene. In this study, we developed a CRISPR/Cas13a-mediated SERS-based dual-flow assay strip sensor to detect SARS-CoV-2 RNA directly. Initially, CRISPR/Cas13a reaction occurred through the first channel, followed by the sequential flow of SERS nanotag solution through the second channel. This sequential flow arrangement allows for both the CRISPR/Cas reaction and the SERS assay within a single chip, enabling the sensitive detection of SARS-CoV-2 RNA. Furthermore, by utilizing CRISPR/Cas13a system, direct detection of SARS-CoV-2 RNA is possible without the need for a reverse-transcription process. Consequently, our SERS-based dual-flow paper chip holds significant potential for point-of-care testing (POCT) by enabling the direct detection of target RNA through two distinct reactions within a single chip.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:25

Chair: Yeonho Kim (Konkuk University)

Development of Multifunctional PCM Microcapsules with biocompatibility and Analysis of Physicochemical Characteristics

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Phase-change materials (PCMs) are substances that manage heat through phase transitions, offering significant latent heat for energy storage, making them valuable in construction, textiles, and energy transport. Despite encapsulation techniques mitigating toxicity, leakage, and chemical instability of PCMs, the safety of the encapsulating materials themselves continues to pose significant concerns. In this study, we developed PCM capsule materials with biocompatible and high thermal stability shells that can be used in various fields and analyzed their physicochemical properties. The emulsion polymerization method was used to encapsulate PCM, and Polymethylmethacrylate (PMMA), which has high thermal stability, biocompatibility, and chemical resistance, was selected as the wall material. The morphological structure was confirmed through microscopic images, and the size distribution and PDI were measured by DLS. These results showed the formation of capsule material with an overall uniform size of about 7.8 μm. Also, FT-IR measurements were performed, and the disappearance of C=C peak confirmed change in molecular structure due to polymerization, which indicated that the shell was formed well. To further analyze the structure of the synthesized capsules, we measured the 1D NMR and found that the peak signal of ester group and repeat unit structure of PMMA were identified, confirming that polymerization had occurred, and a specific structure and phase change of core could be assigned. In conclusion, the overall results demonstrated that the PCM capsule successfully formed a core-shell structure, indicating

promising potential for diverse application. Future work will involve evaluating the thermal performance and stability of these capsules using TGA and DSC measurements.

Oral Presentation : **ANAL1.O-16**
Oral Presentation of Young Analytical Chemists I
Room 103+104 THU 10:32
Chair: Yeonho Kim (Konkuk University)

Optimization of lecithin-encapsulated drug delivery system: Comprehensive NMR characterization and improved skin permeation profiles

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Polymeric micelles derived from self-assembled amphiphilic block copolymers represent a new paradigm in drug delivery system (DDS) due to their high delivery efficiency and biocompatibility, which enhance therapeutic efficacy and reduce side effects. This study synthesized a drug carrier (micelle/emulsion) using the amphiphilic polymer PEO-b-PCL and assessed their physiochemical changes via ^1H NMR, contingent on the type and concentration of lecithin additive. By measuring the T_2 relaxation time within these systems, we discerned that incorporating 10% symmetric lecithin into micelles and 10% into emulsions yielded optimal stability. Conversely, the greatest flexibility of micelles and emulsions with asymmetric lecithin was observed at 15% and 5%, respectively. Given these points, NMR-based T_2 relaxation time measurements provided deeper insight into how the structural properties of the additive affect the stability and flexibility of the drug transporter. Moreover, Franz cell assays were conducted on emulsions exhibiting optimal flexibility to confirm their skin penetration efficacy, thereby proving their viability for pharmaceutical applications. After applying the emulsions to the skin for 24 hours, their permeability was quantitatively analyzed by HPLC. In consequence, emulsions containing asymmetric lecithin exhibited significantly higher penetrability than those with symmetric lecithin. Accordingly, overall results demonstrate that core crystallinity, a key factor in the performance of drug delivery vesicles, can be effectively regulated by varying the type and concentration of additives and evaluated

with NMR. These findings contribute the way for designing advanced complex drug carriers, potentially offering strategic insights for improvement.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:39

Chair: Yeonho Kim (Konkuk University)

Investigation on Physicochemical Property and Structure of Human Hair Using ^{13}C Cross-Polarization Magic Angle Spinning NMR Spectroscopy

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Solid-state NMR is the most promising method for structural analysis of complex, solid biological tissues, and cross-polarization was used to increase the peak intensity of carbon. We aimed to investigate specifically the structural and mobility changes in human hair subjected to various cosmetic treatments such as bleaching, perming, dyeing, and straightening. In this study, ^{13}C CP-MAS NMR was performed to analyze the structure of α-keratin, a major component of hair, and $T_{1\rho}$ relaxation time was measured to evaluate the mobility of hair. ^{13}C CP-NMR spectra revealed variations in the metabolite as the number of hair bleaching steps increased. The area and linewidth of α-helix decreased and β-sheet increased in the carbonyl region, and the portion of cysteine decreased due to disulfide bond cleavage in the aliphatic carbon region, which is the side chain of amino acid. By observing clear $T_{1\rho}$ changes in α-helix and β-sheet of the hair, the shorter relaxation time of treated hair in α-helix suggests that the cosmetic procedure resulted in bond breaking and increased mobility. Further, the physicochemical properties of the hair were confirmed by various analytical instruments such as SEM, FT-IR and microscope. Ongoing work is focused on performing principal component analysis to qualitatively assess the condition of hair after chemical treatment. In conclusion, we would like to propose a new approach to develop an evaluation method using solid-state NMR and build a database based on it for the comparative analysis of different hair types caused by cosmetic procedures.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:46

Chair: Yeonho Kim (Konkuk University)

Dynamic Nuclear Polarization of Onion-Shaped Silica Nanoparticles with Selective 29Si Isotope and Radical Enrichment

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Silica nanoparticles exhibit favorable attributes for developing 29Si MRI probes, featuring advantageous dispersion, biocompatibility, tunable size, and facile surface modification. However, challenges arise in detecting low-concentration species and low-γ nuclei using magnetic resonance spectroscopy. To address this, we explore the application of the Dynamic Nuclear Polarization (DNP) technique, known for amplifying NMR signals, however, the successful hyperpolarization with SiO2 NPs is hindered by the lack of intrinsic electronic defects. In this study, we introduce diverse onion-shaped SiO2 NPs (40 nm core@10 nm shell@10 nm shell) with selective 29Si isotope and TEMPO radical enrichment in distinct regions. The increased 29Si ratio enhances the magnetic resonance signal, and the embedding of free radicals facilitates particle polarization. Through detailed experiments, we establish the potential for self-polarization in DNP, advancing the development of SiO2-based 29Si MRI probes.

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

Oral Presentation of Young Analytical Chemists I

Room 103+104 THU 10:53

Chair: Yeonho Kim (Konkuk University)

Development of Light-Responsive Polylactic Acid for Sustainable Biodegradable Materials: Synthesis and Microcapsule Formation

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The escalating environmental impact of petrochemical-derived plastics and their subsequent accumulation in ecosystems have necessitated the exploration of biodegradable alternatives derived from renewable sources. Polylactic acid (PLA) has emerged as a promising candidate due to its renewable, biocompatible, and biodegradable nature. To advance the application of this polymer, our study aimed to develop PLA as a stimuli-responsive polymer (AZO-PLA) by incorporating a photo-switchable monomer (azobenzene, AZO) into the long-chain polymer. The light-switchable microcapsules were fabricated using a precipitation method afterward. The structures of PLA and AZO-PLA were characterized by 1H, 13C, and DOSY NMR spectroscopy. Results from 1H NMR and polymer end-group analysis confirmed the successful fabrication of low-molecular-weight (L)-PLA from lactic acid monomers. Furthermore, the attachment of light-responsive monomers to the PLA chain was validated by the appearance of aromatic signals in the NMR spectra of AZO-PLA. SEM and NMR techniques were employed to characterize the formation of microcapsules based on AZO-PLA, demonstrating the creation of small spherical capsules from the synthesized polymers. Future research will investigate the light-responsive properties influencing the structure of both polymers and capsules using UV-Vis and NMR analysis.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 09:00

Chair: Hongki Kim (Kongju National University)

Probing Optical Characteristics and Chemical Interface Damping in Gold Nanorods via Cucurbit [6] uril Host-Guest Chemistry

Ji Min Kim, Ji Won Ha[*]

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Gold nanoparticles (AuNPs) have attracted considerable attention in various fields due to their excellent compatibility with living organisms and stable chemical properties. They are particularly useful for facilitating processes like chemical interface damping (CID) when they interact with molecules adsorbed onto their surface. Despite their potential, research using host-guest supramolecular systems to control CID on AuNPs has been limited. This study introduces a new method for controlling CID on AuNPs using host-guest supramolecular complexes. We created a complex called CB[6]-BAPA, based on a well-known host molecule called Cucurbit [6] uril (CB[6]), which has the ability to encapsulate and release guest molecules. By employing this complex, we were able to modulate CID processes on AuNPs in a reversible manner. Through a series of experiments, we demonstrated how the CB[6]-BAPA complex could be used to control CID. By attaching amine groups from the complex onto gold nanorods (AuNRs) and then releasing CB[6] using an alkaline solution, we achieved precise control over the CID process. Changes in certain parameters during the experiments confirmed the successful formation of the CB[6]-BAPA complex and the release of CB[6]. Therefore, this study provides new insights and potential applications, such as in biosensing and drug delivery, by showing how reversible control of CID can be achieved using CB[6]-based host-guest complexes on individual AuNPs.Keywords: gold nanorods, localized surface plasmon resonance, chemical interface damping, cucurbit [6] uril, host-guest.

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Oral Presentation : **ANAL2.O-2**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 09:06
Chair: Hongki Kim (Kongju National University)

Unraveling Plasmon Damping in Silver–Coated Gold Nanorods: Insight from Single–Particle Analysis and Damping Tuning

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A study about silver–coated gold nanorods (AuNR@Ag) remains a captivating area of research. In this study, the morphology and optical properties of AuNR@Ag is investigated. We examined the relation between surface damping and the thickness of silver shell on a single particle level. Utilizing Scanning Electron Microscope (SEM) and Dark Field (DF) Spectroscopy, we studied the near-infrared longitudinal peak in AuNR. We aim to finely adjust the bulk damping and radiation damping of AuNRs to understand the role of surface damping better. Notably, we observe visual changes in gold nanorods upon silver coating, accompanied by an increase in incubation time. SEM analysis reveals an increase in length and width following silver deposition. Energy-dispersive X-ray spectroscopy (EDS) confirms the deposition of silver with increasing content in a longer incubation time. DF Spectroscopy shows a distinctive blue shift and slight broadening. Adjustment in surface damping demonstrates a decrease with an increase in silver content. This study enhances our understanding of the interaction between silver and gold the interface

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 09:12

Chair: Hongki Kim (Kongju National University)

Study Competition between Plasmon Decay pathways of Gold Nanorods on Graphene

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We present an analysis of the electron transfer during interaction of gold nanorods with graphene layered on glass. Using single -particle dark field microscope we tried to observe surface plasmon resonance for gold nanorods and resulting broadening on full width half maximum of gold nanorods. This condition assigns that plasmon damping to charge transfer between plasmon generated hot electrons and the graphene that acts as efficient acceptor. Then we also tried to study the interaction of gold nanorod on graphene with pyridine. Where pyridine can cause plasmon damping on gold nanorods surface. Interestingly, we found that narrowing of the surface plasmon resonance for gold nanorods exposed graphene and pyridine. This result present competition of charge transfer for gold nanorods when interacting with graphene and pyridine.

Oral Presentation : **ANAL2.O-4**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 09:18
Chair: Hongki Kim (Kongju National University)

Electrochemical Tuning of Hot-electron Generation and Chemical Interface Damping in Single Gold Nanorods

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Gold nanoparticles (AuNPs) exhibit the localized surface plasmon resonance (LSPR) property, which refers to the collective oscillation of conduction band free electrons when interacting with the electromagnetic spectrum. Gold nanorods (AuNRs), which have tunable size, shape, and structure-dependent plasmonic properties, experience LSPR energy loss when the organic molecules absorb onto their surface. This phenomenon of LSPR energy is called chemical interface damping (CID). The change in the dielectric constant of the surrounding medium due to organic molecule adsorption may result in LSPR peak shift, intensity variations, and linewidth change, which can be examined at the single-particle level. The AuNRs having biocompatible, photostable, and electrically conductive properties enable the possibility of combining spectroscopy with electrochemistry. Single-particle spectroelectrochemistry that combines single-particle dark field scattering-based (DFS) microscopy and spectroscopy with an electrochemical workstation made possible the electrochemical plasmonic sensing and tuning of the chemical interfaces at the single-particle level. AuNRs of the desired size (25 × 75 nm) were immobilized on indium tin oxide (ITO) substrates to construct plasmonic electrodes for this investigation. In this study, we discuss the CID effect induced by thiol molecule adsorption onto the AuNR surface. The effect of electrochemical manipulations at the bare AuNRs and the gold-thiol interface was examined. Electrochemical tuning of LSPR energy loss (or CID) at the interface of Au-thiol and its effects on the stability of thiol molecules on the Au surface was analyzed by probing the LSPR energy shift, change in

peak intensity, and linewidth change for time-dependent and potential-dependent variations at the single-particle level.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 09:24

Chair: Hongki Kim (Kongju National University)

Performance evaluation of thickness-tapered channel in flow field-flow fractionation with the effect of field programming in a uniform channel

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Flow field-flow fractionation (flow FFF) is a method employed for separating particulate materials based on particle sizes. Particles traverse a thin rectangular channel space with a carrier liquid, while crossflow, applied perpendicular to the channel axis, serves as the driving force for separation. To enhance the separation efficacy of flow FFF, field programming with a flow controller has been introduced, enabling varying crossflow rates over time to achieve lower retention times and improved separation performance. However, integrating a flow controller for field programming adds to the overall cost, prompting the need for a novel flow FFF technique capable of enhancing separation performance without altering flow rates.The introduction of a thickness-tapered channel in flow FFF presents a solution to this challenge, employing a channel with decreasing thickness along its length. This study directly compares the separation performance of the thickness-tapered channel with that of a conventional asymmetrical flow FFF channel using field programming. Results demonstrate that the thickness-tapered channel yields comparable separation performance to field programming, enhancing retention time and sample recovery.Continuing the evaluation, the thickness-tapered channel's performance will be assessed in the separation of lipoproteins. Enhanced resolution and sample recovery afforded by the thickness-tapered channel offer the potential for improved separation of low-density lipoproteins (LDL) and very-low-density lipoproteins (VLDL), which pose challenges in conventional flow FFF separations.

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Oral Presentation : **ANAL2.O-6**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 09:30
Chair: Hongki Kim (Kongju National University)

Top-down lipid analysis of exosomes derived DU145 cells using mAF4-ESI-MS/MS

Hyeju Yu, Donggyun Kim, Myeong Hee Moon*

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Extracellular vesicles (EVs) are cell-derived membrane-bound particles, including exosomes and microvesicles, characterized by a lipid bilayer structure. Exosomes (30–150 nm in diameter), which are released by the fusion of multivesicular bodies with the plasma membrane, play an important role in intercellular communication and are expected to serve as useful biomarkers for various diseases. Conventional lipidomic analysis of exosome lipids typically performed through bottom-up analysis using liquid chromatography-tandem mass spectrometry (LC-ESI-MS/MS). This method qualitatively and quantitatively analyzes total lipids by extracting the lipidome from biological sources with organic solvents. This study aims to demonstrate the potential of top-down analysis by miniaturized asymmetrical flow field-flow fractionation and electrospray ionization-tandem mass spectrometry (mAF4-ESI-MS/MS) as a high-speed screening platform for direct analysis of exosomes from the culture media of DU145 cells without extraction. Using an mAF4 channel, exosomes can be separated at high speeds (

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 09:36

Chair: Hongki Kim (Kongju National University)

SARS-CoV-2 induced lipid perturbation in lung, liver, and serum of mice

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The emergence of SARS-CoV-2, the virus responsible for COVID-19, has presented a significant danger to public health worldwide. COVID is characterized by symptoms such as tiredness, coughing, tightness in the chest, shortness of breath, palpitations, muscle pain, and difficulty with concentration. These symptoms may be associated with various conditions, such as damage to organs, syndrome following a viral infection, syndrome following critical care, and other related conditions. Lipids serve as both a source of energy and as essential components of cells, while also playing a crucial role in cellular signaling pathways and regulating the permeability of cell membranes. Therefore, metabolic alterations may result in changes in lipid composition and its level. In this study, the recovery process from the infection of COVID-19 will be observed in the lung, liver, and serum of K18-hACE2 mice by monitoring changes in lipid composition using nUHPLC-ESI-MS/MS. A total of 703, 869 and 466 lipids were identified in the lung, liver and serum samples from mice through qualitative analysis. At 1x10^2 PFU/mL (plaque forming unit), most lipid classes exhibited substantial decreases in lung tissue at 2 days post-infection (dpi), followed by subsequent recovery. Similarly, at 1x10^5 PFU/mL, most lipid classes showed significant reductions in lung tissue at 1 dpi, followed by subsequent recovery. However, TG (Triacylglycerol) showed a steady decreasing trend in lung tissue. Even in liver, most lipid classes decrease and then recover. Qualitative and quantitative analysis is being conducted to assess the degree of

recovery in mice infected with COVID-19. This study will contribute to the understanding of organ damage and recovery resulting from COVID-19 infection.

Oral Presentation : **ANAL2.O-8**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 09:42
Chair: Hongki Kim (Kongju National University)

Optimization of skin sampling method for lipidomic analysis by nanoflow UHPLC-ESI-MS/MS

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The human skin serves as the primary physical barrier against the external environment, with the outermost epidermal layer, known as the stratum corneum, composed of lipids such as ceramides and glycerolipids. Tape stripping is a common method for skin sampling, involving the use of adhesive tape to collect stratum corneum layers. Due to various factors influencing lipid removal by each tape strip, a standardized sampling procedure is essential. This study aimed to optimize skin sampling method in terms of sampling location and the number of tape strips during repeated stripping. Skin samples were obtained from seven sequential tape strips taken from the same spot and from four different locations (forehead, forearm, cheek, and neck). Lipid analysis was followed by nanoflow ultrahigh performance liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS). Lipid profiles were analyzed by comparing the normalized peak area of individual lipid species relative to the peak area of internal standard specific to each lipid class. When skin samples were repeatedly taken from the same spot, the number of identified lipid species tended to decrease, which became significant after the 6th layer. To overcome the layer to layer variation in lipid composition, a pooling method of different tape strips was adopted. Extracts from the first 3 or 5 consecutive layers were pooled, respectively, and analyzed. This approach resulted in the identification of over 50 additional lipid species in the pooled samples compared to individual tape strip extracts. Prior to optimizing the number of tape strips for sample pooling, the variation in lipid composition and quantities among adjacent spots was evaluated. From statistical comparison of quantified results, the normalized peak area of each lipid species from the

three adjacent spots were not statistically different from each other. Therefore, sample pooling was adopted to establish the most representative tape stripping method that accurately reflects skin lipid composition and avoid loss of quantifiable lipids.

Oral Presentation : **ANAL2.O-9**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 09:48
Chair: Hongki Kim (Kongju National University)

Lipid alternations in brain and spleen tissues of SARS-CoV-2 mouse using nanoflow UHPLC-ESI-MS/MS

Hwangyu Park, Myeong Hee Moon[1,*], Soomin Kang[2]

Department of chemistry, Yonsei University, Korea
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[2]Yonsei University, Korea

Various corona virus diseases including SARS and MERS, along with SARS-CoV-2, have been prevalent in the 21st century, posing ongoing concerns due to continuous mutation. Therefore, research is increasingly needed due to similarities in symptoms, infection, and metabolic pathways among betacoronaviruses.Lipids play a critical role in viral entry, replication, and assembly and are involved in many pathological symptoms. Hence, the accumulation of lipidomic research data can aid in early diagnosis and treatment strategies.To evaluate the impact of varying doses of SARS-CoV-2 on spleen and brain tissues over time, this study conducted qualitative and quantitative lipidomic analyses at six different time points. Mice were infected with two different levels of plaque-forming units (PFU), and their tissue lipids were analyzed in comparison to control group.In this study, we examined the lipid profiles of SARS-CoV-2-infected mice in both spleen and brain tissues using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry. Through this comprehensive non-targeted analysis, we identified a total of 593 and 926 lipids in the brain and spleen tissue, respectively. Remarkably, targeted quantification unveiled significant changes in the majority of lipids within the infected group, regardless of the infection dosage.Most of Phospholipids displayed a consistent decreasing trend in both brain spleen and brain tissues. On the other hand, sphingolipids (SLs) exhibited a notable increase in brain. But SLs show opposite trends in the spleen. Specifically, alterations were observed in the ratio between phosphatidylcholine and phosphatidylethanolamine, both prevalent in cell membranes. Notably, this ratio exhibited a trend towards recovery beginning on the 7th day after infection. A thorough statistical analysis will be provided.

Oral Presentation : **ANAL2.O-10**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 09:54
Chair: Hongki Kim (Kongju National University)

Advanced 19F NMR Investigation of Poly (vinylidene fluoride) (PVDF) Crystalline Phases for Good-performance Electrode

Jae Hwa Choi, SeokKi Yun, Seyoung Yang, Quy Son Luu, Youngbok Lee[1,*]

Hanyang University, Korea
[1]*Department of Bio-Nano Engineering, Department of, Hanyang University, Korea*

With the growing demand and interest in lithium batteries in energy storage fields such as electric vehicles, smartphones, laptops, etc., research on binders, one of the important components of lithium batteries, has also increased. PVDF, known for its versatility as a dielectric polymer, exhibits four distinct crystalline phases: α, β, γ, and δ. Existing research has predominantly examined PVDF's binder efficacy through surface and electrochemical analyses, yet a comprehensive understanding of its behavior during battery cycling and the impact of its polymorphic nature remains underexplored.In this study, NMR analysis and IR analysis were conducted as an analysis method to determine the PVDF's crystallinity that affects battery performance.Initial phase of the research involved segregating commercial PVDF samples into their α and β phases via recrystallization techniques, and a series of 1H, 19F solution-state NMR experiments on the α and β films were conducted to delve into their structural and dynamic properties. Detailed structural properties of the PVDF materials were examined, however, phase information of the recrystallized phase was lost in the solution NMR measurements. To address this, solid-state 19F and 13C NMR experiments were conducted and phase transition issues of the PVDF were overcome in the advanced solid-state methodology. The outcomes of this research underscore the effectiveness of NMR-based method in accurately determining the intricate molecular structure and crystallinity of PVDF binders. These attributes have a direct and significant impact on the performance of electrodes in lithium-ion batteries, highlighting the crucial role of advanced material analysis in the progression of energy technologies.

Oral Presentation : **ANAL2.O-11**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 10:00
Chair: Hongki Kim (Kongju National University)

Investigation on Raman spectral features according to variation of internal thickness of pearls

Juyoung Park

Chemistry, Hanyang University, Korea

Cultured pearls are produced by the secretions of shellfish that leading to form a thin film of artificial nuclei in the body and layers. Aragonite (calcium carbonate, $CaCO_3$) and conchiolin (protein) form a layer outside the nucleus, and are being stacked during the growth. This multi-layered structure, called the Nacre layer, determines the gloss and size of pearls, and is the factor that directly influences on the commercial value of pearl. However, it is difficult to estimate the internal thickness of the pearl layer, and only feasible when a pearl is cut for naked-eye examination. Therefore, a non-destructive analytical method for this purpose is critically required and Raman spectrscopy providing sensitive spectral information on the constituents of pearl is surely a candidate. Initially, the differences in the Raman spectra of Akoya pearls cultivated in the three countries (China, Japan, and Korea) were investigated. Next, since the Nacre layer is mostly composed of calcium carbonate, the intensities of corresponding peaks were examined and discussed in relation with the internal thickness of the Nacre layer.

Oral Presentation : **ANAL2.O-12**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 10:06
Chair: Hongki Kim (Kongju National University)

Urinary metabolic profiling in ECMO-treated severe COVID-19 patients

Sunho Lee, Youngae Jung, Geum-Sook Hwang[1,*]

Metropolitan Seoul Center, Korea Basic Science Institute, Korea
[1]*Korea Basic Science Institute, Korea*

Coronavirus (COVID-19) emerged in 2019 and continues to persist to this day. In severe cases of infected patients, extreme lung inflammation and damage may result in inadequate oxygen supply, necessitating extracorporeal membrane oxygenation (ECMO) therapy. In this study, we observed changes in urine metabolites following ECMO treatment, based on survival outcome and the presence of diabetes, using liquid chromatography tandem mass spectrometry (LC-MS/MS). We collected urine samples from 25 severe COVID-19 patients who received ECMO therapy in 2021 and 2022. These samples comprised 10 from deceased patients and 15 from survivors. Additionally, we categorized the samples based on the presence of diabetes, with 18 samples from non-diabetic patients and 7 from diabetic patients.As a result of multivariate analysis, partial least squares discriminant analysis (PLS-DA) score plots were generated using quantified 70 metabolites, showing separation based on survival and diabetes status. In metabolic profiling, elevated levels of ADMA, arginine, citrulline, folic acid, iso-carnitine, and nicotinamide were observed in deceased patients relative to survivors. And adenosine, ADMA, betaine, but-carnitine, folic acid, N-acetylglutamic acid, pyroglutamic acid, and TMAO were found to be elevated in diabetic patients compared to non-diabetic. These findings demonstrate the substantial metabolic alterations induced by COVID-19 infection. This study offers valuable insights of the utility of LC-MS/MS-based metabolomic analysis for observing urinary metabolites in severe COVID-19 patients.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:12

Chair: Hongki Kim (Kongju National University)

Defects healing of the ZnO surface by filling with metal atom catalysts for boosting solar hydrogen production

Jiyoung Bae, Yeonho Kim*

Department of Applied Chemistry, Konkuk University, Korea

Healed defects on photocatalysts surface and their interaction with plasmonic nanoparticles (NPs) have attracted attention in H2 production process. In this study, surface oxygen vacancy defects are created on ZnO (Vo-ZnO) NPs by directly pyrolyzing zeolitic imidazolate framework. The surface defects on Vo-ZnO provide active sites for the diffusion of single Au atoms and as nucleation sites for the formation of Au NPs by the in-situ photodeposition process. The electronically healed surface defects by single Au atoms helped in the formation of a heterojunction between the ZnO and plasmonic Au NPs. The strategy for the direct deposition of metal atoms on the submain surface of the semiconductor without binder and healed defect by filling single metal atoms could be advantageous for the prolongs photoelectron lifetimes and increasing donor charge density. Therefore, the optimized photocatalysts shows enhanced H2 production under UV-visible and visible light. Furthermore, Au/Vo-Au:ZnO shows visible light activity by generating hot carries via induced surface plasmonic effects. Therefore, this study inferred new insight for defect healing mediated preparation of Au/Vo-Au:ZnO heterojunction for efficient photocatalytic H2 production.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:18

Chair: Hongki Kim (Kongju National University)

Lipidomic changes of brain tissue in an Alzheimer’s disease mouse model overexpressing Tau

Su-Hyun Chae, Jueun Lee, Do Hyun Ryu[1,*], Geum-Sook Hwang[2,*]

Metropolitan Seoul Center, Korea Basic Science Institute, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*
[2]*Korea Basic Science Institute, Korea*

Alzheimer's disease(AD), the most common neurodegenerative brain disease that causes dementia, has been reported to have a steadily increasing incidence rate worldwide, but its therapeutics is not clearly defined. Abnormal accumulation of tau aggregates is considered a common pathological feature of Alzheimer's disease. However, research on the mechanisms underlying tau pathology associated with aberrant lipid metabolism within brain tissue are poorly understood.To evaluate the lipidomic changes in relation to Tau pathology, we performed lipidomic analysis of the brain tissues of PS19 wildtype mice aged 4.4-months and 11-months and human tau-overexpressing PS19 mice aged 4.4-months(early-stage AD) and 11-months (late-stage AD) using ultra performance liquid chromatography trapped ion mobility spectrometry time-of-flight mass spectrometry(UPLC TIMS-TOF MS). As a result of multivariate analysis, the score plot of principal component analysis showed a clear separation between the wild-type and Tau group at 11-month, stronger than at 4.4-month indicating significant alterations in the lipidomic profiles of the brain tissue from tau mice at 11-month. Specifically, in the late-stage tau group, the levels of cholesteryl ester, ceramide, triacylglycerol, and phosphatidylglycerol were significantly increased compared to the other groups.Therefore, our findings suggested that the alterations in lipid metabolism in the brain due to tau aggregation have a comparable between 4.4-month-old wildtype and early-stage AD, but reveal significant lipid accumulations as the disease progresses to late-stage AD. This study also

demonstrated that lipidomic analysis using TIMS-TOF MS is a useful method to investigate lipid metabolism associated with Tau pathology and Alzheimer’s disease.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:24

Chair: Hongki Kim (Kongju National University)

Metabolomics time-course response in liver tissues after SARS-CoV-2 infection

Yejin Bae, Youngae Jung[1], Geum-Sook Hwang[2,*]

Metropolitan seoul center, Korea Basic Science Institute, Korea
[1] *Western Seoul Center, Korea Basic Science Institute, Korea*
[2] *Korea Basic Science Institute, Korea*

SARS-CoV-2 infects the nasopharynx and lungs, however, several studies have reported cases of acute liver injury and liver failure following SARS-CoV-2 infection. Moreover, changes in liver metabolism caused by SARS-CoV-2 have not been clearly identified. In this study, liver tissue was collected from hACE2 mice model (n = 57) intranasally infected with 10^2 Wuhan virus at 2, 5, 7, 14 days post-infection (dpi) and control group (no infection). Analysis of liver tissue from SARS-CoV-2 infection mice was performed by untargeted metabolomics approach using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS). Clustering analysis based on 67 significantly changed hepatic metabolites after SARS-CoV-2 infection was performed to identify trends in metabolic changes in the liver, and three clusters were generated. In Cluster1, metabolite levels showed an increasing tendency after 2 and 5 dpi. In particular, significant changes could be observed in acyl-carnitines and amino acids levels, suggesting metabolic changes in response to early inflammation. Cluster2 displayed a rise in metabolite levels post 7 dpi. Notably, citrulline and dimethylglycine, elevated in severe coronavirus infection. Conversely, Cluster3 exhibited a tendency towards decreased metabolite levels in the infection group, with NAD+ gradually decreasing from 2 dpi to 14 dpi. This study demonstrated that hepatic metabolites has changed according on the time points during SARS-CoV-2, and LC/MS-based metabolomics may provide insight into metabolic pathway involved in liver dysfunction in SARS-CoV-2 infection.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:30

Chair: Hongki Kim (Kongju National University)

Advancing Analytical Strategies for the Comprehensive Detection and Quantification of Cyclic Imines in Marine Ecosystems

Hyewon Kim, Hyun Joo An*

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

Rapid changes in the marine ecosystem have brought attention to emerging toxins such as Cyclic Imines (CIs), posing a significant risk. Indeed, cases of exposure to the risk of CI toxicity are continuously reported in various European countries, but the absences of established international standards hinders effective management. CI analysis present challenges due to the limited availability of commercial standards (only seven out of more than 40 reported analogues) and their presence at very low concentrations in marine organisms along with numerous interfering lipophilic substances. In this study, we developed a multi-step platform to simultaneously identify and quantify CI analogs encompassing extraction, purification, analysis, and data interpretation. In particular, the development of an in-silico library capable of predicting elution time and MS/MS pattern is noteworthy. This predictive capability is based on the commercialized CI series including 3 types SPX, 1 type GYM, and 3 types PnTX. Using this platform, we successfully monitored CI isomers in approximately 400 species of shellfish collected from the Korean Peninsula over a span of 4 years. Note that PnTX G (4.131~14.42 pg/g), GYM A (21.23~309.9 pg/g), and 13-desMe SPX C (4.502~15.19 pg/g) were detected for the first time in about 110 species. Detected CI concentrations exhibited a positive correlation with increasing sea surface temperature. By applying this innovative analysis platform in real-world marine ecosystems, our approach holds promise for the ongoing monitoring and safety management of marine biological toxins.

Oral Presentation : **ANAL2.O-17**
Oral Presentation of Young Analytical Chemists II
Room 103+104 FRI 10:36
Chair: Hongki Kim (Kongju National University)

Characterization of self-assembled micelle inhibitory RNA drug using ion-pairing reversed-phase liquid chromatography combined with mass spectrometry

Hyojin Hwang, Jeongkwon Kim[1,*]

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

Oligonucleotide drugs are promising therapeutics for various diseases, driving significant research efforts towards their development and enhancement. The conventional siRNA drugs have limitations in delivery efficiency, to address this, SAMiRNA, which combines hydrophilic and hydrophobic groups at both ends of the sense strand, has been developed. Given the heavy chemical modifications in SAMiRNA, its behavior in ion-pairing reversed-phase liquid chromatography (IP RPLC) combined with mass spectrometry (MS) is expected to differ from that of conventional siRNA drugs. Therefore, the development of appropriate analytical methods is warranted. The composition of ion pairing reagent in the buffer system directly affects chromatographic separation and sensitivity of detection by ultraviolet spectrometer and mass spectrometer. This study investigates various ion pairing reagents' effects on oligonucleotide LC systems and enhances method reliability through reproducibility experiments. Dibutylamine, paired with 1,1,1,1,3,3,3-hexafluoro-2-propanol, was employed, with separation on a C18 column, and LC-MS spectra were obtained using a Q-Exactive Plus mass spectrometer. In addition, SAMiRNA was analyzed at seven different column temperatures to observe the duplex form. Below 40 ^{o}C, the duplex peak was detected. Simultaneously, at the retention time of the duplex, antisense and sense strand peaks were observed. The behavior of the SAMiRNA duplex form more closely resembled that of the sense strand than the antisense, likely due to the presence of hydrophilic and hydrophobic groups at both ends of the sense strand.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:42

Chair: Hongki Kim (Kongju National University)

Photo-reversible tuning of chemical interface damping in single gold-nanorods with cucurbit[n]uril and aminoazobenzene

Jaeran Lee, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Photoresponsive molecules are well known as photoswitches because of their reversible changes in structural, electrical, and optical properties in response to photon stimulation. Among the photoresponsive molecules, azobenzene is characterized by photoisomerization, which changes from trans to cis form under UV irradiation. This photoisomerization of azobenzene has been widely studied to develop novel nanoswitches and electronic devices in combination with plasmonic nanoparticles. In this study, we have measured the chemical interface damping of gold nanoparticles due to the photoreactivity of azobenzene molecules upon attachment of cucurbit[n]uril hydrate molecules accepting aminoazobenzene to the surface of single gold nanorods. Among the various cucurbit[n]urils, we used cucurbit[6], cucurbit[7], and cucurbit[8], which have sufficient cavities to accommodate aminoazobenzene molecules. We found that aminoazobenzene generally leads to a greater damping effect of gold nanoparticle attachment in the trans form, but the aminoazobenzene cavity-accommodated in cucurbit[n]uril has more damping effect in the cis form. This work will provide insight into understanding how aminoazobenzene acceptance in supramolecules such as cucurbit[n]uril affects photoreversible molecular reactions.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:48

Chair: Hongki Kim (Kongju National University)

Electrochemical Impedance Spectroscopy Analysis for Non-destructive Determination of Compressive Strength of Concretes

Junhee Yu, Hyun Ju Yang, Hyo Chan Lee, Je Hyun Bae*

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

To date, methods used to assess the interfacial transition zone (ITZ), which represents the boundary between the aggregate and paste inside concretes, have primarily relied ondestructive tests, and non-destructive tests has received little attention until recently. This study assessed the interfaces of concretes with lightweight aggregates based on electrochemical impedance spectroscopy (EIS) for high-strength concretes and examined the possibility of estimating the compressive strength of concretes through non-destructive testing using EIS. The experimental results revealed that the impedance of the hardened cement increased with increasing compressive strength and aggregate density. In particular, when the results of impedance measurement were displayed as a Nyquist plot, the intercept of the x-axis depicting the effective conductivity was proportional to the compressive strength. Furthermore, an equivalent circuit was selected to interpret the correlation between cement aggregates and impedance. Consequently, the compressive strength was found to increase with the value of the resistances of the electrolyte filled in continuous pores in the cement aggregate. And, the pores formed in the ITZ affect this value. The resistance at the ITZ for different aggregates was also obtained, and it was found that the resistance was consistent with the results predicted by SEM images of the ITZ and correlated with the strength of the concretes. The proposed method can be used as a way to easily determine the strength of cement according to differences in aggregate.

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

Oral Presentation of Young Analytical Chemists II

Room 103+104 FRI 10:54

Chair: Hongki Kim (Kongju National University)

Comprehensive Characterization of Brain Gangliosides from Alzheimer’s Disease Mouse Model using Chromatographic Separation and Tandem Spectral Library Matching

JongHyun Yoon, Hyun Joo An[1,*]

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

[1]*Graduate School of Analytical Science and Technolo, Chungnam National University, Korea*

Gangliosides, which make up less than 1% of the total brain, are important components involved in nerve growth and development, neurotransmitter transport, and prevention of cell death. Recent research has notably focused on the potential of gangliosides in the diagnosis, treatment, and prevention of brain-related disease such as Alzheimer's disease (AD). However, the analysis of gangliosides is challenging due to their complex structure, characterized by a ceramide lipid tail and a glycan head group.. Here, we developed an LC/MS-based platform for the comprehensive characterization of brain gangliosides and observed changes associated with AD. First, we efficiently isolated complex gangliosides from brain tissue using a C18 column, which is mainly influenced by lipid composition. Then, structure-specific b-/y-ions such as m/z 454 ([Hex+Neu5Ac+H]+), 583 ([2Neu5Ac+H]+) and 657 ([Hex+HexNAc+Neu5Ac+H]+) were monitored to assign isomers with different positions of the terminal sialic acid. Our LC/MS-based data interpretation strategies enabled the comprehensive characterization of gangliosides through the integration of structure-based MS/MS spectra and RT predictions. To facilitate interpretation, we utilized the Personal Compound Database and Library program to construct a meticulously curated database, systematically cataloging compound details such as formula, exact mass, and RT. Indeed, we successfully characterized 79 ganglioside compounds extracted from representative five regions in AD model and normal mouse brain. Furthermore, the identification and quantitative comparison of isomers such as GD1a/b allowed for the prediction of ganglioside synthetic pathways. This analysis revealed significant changes in major gangliosides, including GT1b in the hippocampus, comparing changes across the olfactory bulb, hippocampus, cortex, thalamus, and cerebellum, revealing. Our strategies offer a valuable reference for LC-MS-based ganglioside studies, facilitating comprehensive analysis and understanding in various biological samples.

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Award Lecture in Division : **LIFE.O-9**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 101+102 THU 10:20
Chair: Yong Woong Jun (KAIST)

AbClick: A site-selective antibody conjugation linker platform for off-the-shelf antibodies

Sang Jeon Chung

College of Pharmacy, SungKyunKwan University, Korea

Enhancing the therapeutic potential of antibody-drug conjugates (ADCs) through precise site-selective antibody conjugation has become a revolutionary pursuit in the realm of targeted anticancer therapies. Traditional methods of antibody conjugation, typically relying on Lys and reduced Cys residues, result in complex mixtures of products with variable drug-antibody ratios (DARs) and diverse conjugation sites. While site-directed mutagenesis has enabled site-specific antibody conjugation, it still is impractical for off-the-shelf antibodies.To tackle this challenge, we have developed AbClick®, an innovative site-selective antibody-cross linker which selectively acylates the ε-NH2 group of K248 on off-the-shelf antibodies. AbClick® achieves unparalleled selectivity through a novel approach involving an IgG Fc-binding peptide (FcBP) fused with active esters. Leveraging this cutting-edge linker, we have successfully developed an ADC targeting claudin 18.2, seamlessly incorporating the potent microtubule inhibitor MMAE with a DAR of 2. Our meticulously prepared ADC has proven in vitro anticancer activity comparable to or surpassing that of unmodified MMAE. Moreover, it has shown exceptional in vivo anticancer efficacy in an SNU601 xenograft mice model, with a minimum effective dose (MED) range of 1.0 to 1.5 mg/kg.Extensive toxicity studies in monkeys have provided reassurance, with complete recovery from toxicological symptoms observed within 8 weeks after the last drug administration at doses up to 10 mg/kg. This symposium will provide a comprehensive overview of the AbClick® technology, along with a brief discussion of its successful business applications.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 101+102 THU 09:00

Chair: Yong Woong Jun (KAIST)

DOM: *Dual Optical Mapping* Combining Sequence-Specific Markers and A/T Frequency-Dependent Profiles

Jaeyoung Bae, Kyubong Jo[*]

Department of Chemistry, Sogang University, Korea

We introduce Dual Optical Mapping (DOM), a method that combines sequence-specific barcode-like markers with AT frequency profiles. Optical Mapping has traditionally used barcodes generated by sequence-specific enzymes such as restriction endonucleases, nickases, or methyltransferases. This approach has been commercialized for genomic science applications. In addition, several AT frequency-dependent profiling approaches have been developed, including our prior work on fluorochrome-labelled pyrrole-octamers. Understanding the complementary capabilities of these methods, we conceived DOM, combining sequence-specific barcodes with AT frequency profiles. For efficient alignments, we developed a software tool, DOM.py, that automatically calculates cross-correlation values while considering DNA stretching. This program includes two established optical mapping tools, Maligner and OMBlast, facilitating a comparison of our cross-correlation results. To construct a precise reference map, we performed a computer simulation, postulating that a pyrrole-octamer would preclude neighbouring bindings when bound to an AT-specific site. Using DOM.py with a simulated reference map, we applied DOM to the E. coli genome (4.6 Mbp) as a representative model. We isolated single-molecule images of 182 DNA molecules exceeding 100 kb in length, with 178 of them aligning to the genome in 5.9× coverage. This remarkable alignment rate (98%) demonstrates our confidence in the capability of DOM to align single-molecule DNA images with reference genomes. Consequently, this work highlights DOM's potential for accurately interpreting single-molecule optical mapping DNA images.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 101+102 THU 09:10

Chair: Yong Woong Jun (KAIST)

High-resolution mapping of α-synuclein phosphorylation using single-molecule fluorescence

Moon Hyeok Choi, Chirlmin Joo*

Department of BioNanoScience, Delft University of Technology, Netherlands

α-synuclein is a protein mainly found in the brain. It plays a crucial role in neurodegenerative diseases like Parkinson's. It is known to form abnormal aggregates within neurons, disrupting cellular processes, and impairing synaptic function. The physiological function of α-synuclein is modulated by phosphorylation, which alters its structure, interactions, and cellular roles. Studying the effects of phosphorylation on the structure and function of α-synuclein will deepen our understanding of its biological roles and its dysregulation in disease states. The function of α-synuclein is dependent on the position and number of phosphorylation sites; however, analyzing the profile of multi-phosphorylation remains challenging, necessitating high-sensitivity techniques. Single-molecule biophysics offers exceptional sensitivity in the analysis of individual protein molecules, revealing hidden dynamics and interactions inaccessible to traditional biochemical measurements. We utilize single-molecule FRET (Förster resonance energy transfer) techniques to determine distances between detection spots and create fingerprinting maps to assess the number of sites of interest. We combine this technique with site-specific labeling of phosphorylation, enabling high-resolution mapping of α-synuclein phosphorylation at the single-molecule level.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 101+102 THU 09:20

Chair: Yong Woong Jun (KAIST)

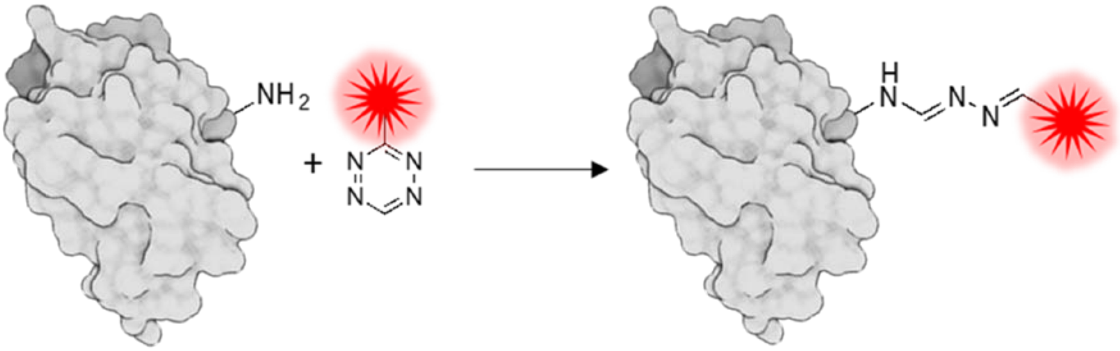
Investigation of proteome-tetrazine reactivity for a minimal background biorthogonal click reagent in live cell.

Junyoung Park, Eunha Kim[1,*], Jongmin Park[*]

Department of Chemistry, Institute for Molecular Science and Fusion Technology, Multidimensional Genomics Research Center, Kangwon National University, Korea

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

Tetrazine undergoes Inverse Electron-demand Diels-Alder (IEDDA) reactions with dienophiles, including trans-cyclooctene (TCO). The IEDDA reaction is one of the click reactions known as bioorthogonal and is being used in various ways, such as observing specific proteins in biological systems or using this reaction as a prodrug strategy.Tetrazine is known to be bioorthogonal. However, some studies have reported that tetrazine is unstable depending on the functional group in the biological environment1,2, and Setiz group reported that tetrazine with two methyl esters reacts with nucleophiles such as amines3. Based on these studies, we hypothesize that, depending on the structure, tetrazines can react with nucleophiles present in biological systems. Various tetrazine derivatives were synthesized to investigate reactivity with nucleophiles in the biological environment. Every tetrazine was conjugated with silicon rhodamine(SiR) as a fluorescent dye. Using them, we investigated the reaction between tetrazine derivatives and proteins in live cells or cell lysates. In addition, the effect of tetrazine and protein reactivity on protein fluorescence imaging was investigated through an experiment in which BTK protein was labeled.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Oral Presentation : **LIFE.O-4**

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 101+102 THU 09:30

Chair: Yong Woong Jun (KAIST)

21 Fluorescent Protein-Based DNA Staining Dyes.

Yurie Kim, Kyubong Jo[1,*]

chemistry, Sogang University, United States

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

Fluorescent protein–DNA-binding peptides or proteins (FP-DBP) are a powerful means to stain and visualize large DNA molecules on a fluorescence microscope. We constructed 21 kinds of FP-DBPs using various colors of fluorescent proteins and two DNA-binding motifs. From the database of fluorescent proteins (FPbase.org), we chose bright FPs, such as RRvT, tdTomato, mNeonGreen, mClover3, YPet, and mScarlet, which are four to eight times brighter than the original wild-type GFP. Additionally, we chose other FPs, such as mOrange2, Emerald, mTurquoise2, mStrawberry, and mCherry, for variations in emitting wavelengths. For DNA-binding motifs, we used HMG (high mobility group) as an 11-mer peptide or a 36 kDa tTALE (truncated transcription activator-like effector). Using 21 FP-DBPs, we attempted to stain DNA molecules and then analyzed fluorescence intensities. Most FP-DBPs successfully visualized DNA molecules. Even with the same DNA-binding motif, the order of FP and DBP affected DNA staining in terms of brightness and DNA stretching. The DNA staining pattern by FP-DBPs was also affected by the FP types. The data from 21 FP-DBPs provided a guideline to develop novel DNA-binding fluorescent proteins.

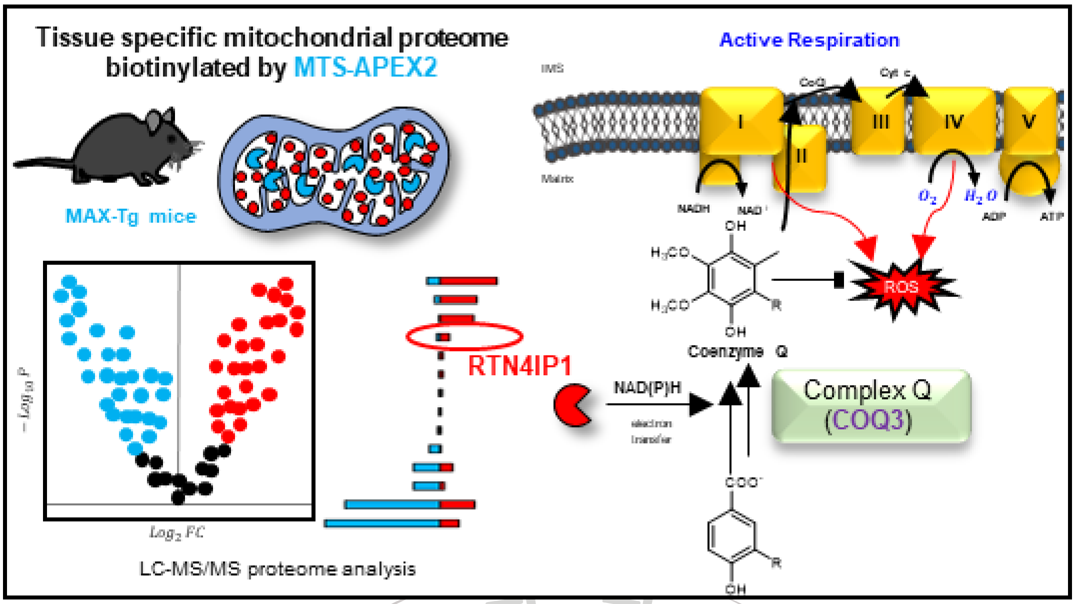
Oral Presentation : **LIFE.O-5**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 101+102 THU 09:40
Chair: Yong Woong Jun (KAIST)

Mitochondrial matrix RTN4IP1/OPA10 is an oxidoreductase for coenzyme Q synthesis

Hyun-Woo Rhee*, Isaac Park[1]

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

Targeting proximity-labeling enzymes to specific cellular locations is a viable strategy for profiling subcellular proteomes. Here, we generated transgenic mice (MAX-Tg) expressing a mitochondrial matrix-targeted ascorbate peroxidase. Comparative analysis of matrix proteomes from the muscle tissues showed differential enrichment of mitochondrial proteins. We found that reticulon 4-interacting protein 1 (RTN4IP1), also known as optic atrophy-10, is enriched in the mitochondrial matrix of muscle tissues and is an NADPH oxidoreductase. Interactome analysis and in vitro enzymatic assays revealed an essential role for RTN4IP1 in coenzyme Q (CoQ) biosynthesis by regulating the O-methylation activity of COQ3. Rtn4ip1-knockout myoblasts had markedly decreased CoQ9 levels and impaired cellular respiration. Furthermore, muscle-specific knockdown of dRtn4ip1 in flies resulted in impaired muscle function, which was reversed by dietary supplementation with soluble CoQ. Collectively, these results demonstrate that RTN4IP1 is a mitochondrial NAD(P)H oxidoreductase essential for supporting mitochondrial respiration activity in the muscle tissue.


Tissue specific mitochondrial proteome biotinylated by MTS-APEX2
MAX-Tg mice
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$Log_2 FC$
LC-MS/MS proteome analysis
RTN4IP1
NAD(P)H
electron transfer
Active Respiration
IMS
Matrix
CoQ
Cyt c
I
II
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IV
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NADH
NAD⁺
O_2
H_2O
ADP
ATP
ROS
OH
H_3CO
H_3CO
R
OH
Coenzyme Q
Complex Q
(COQ3)
COO⁻
R
OH

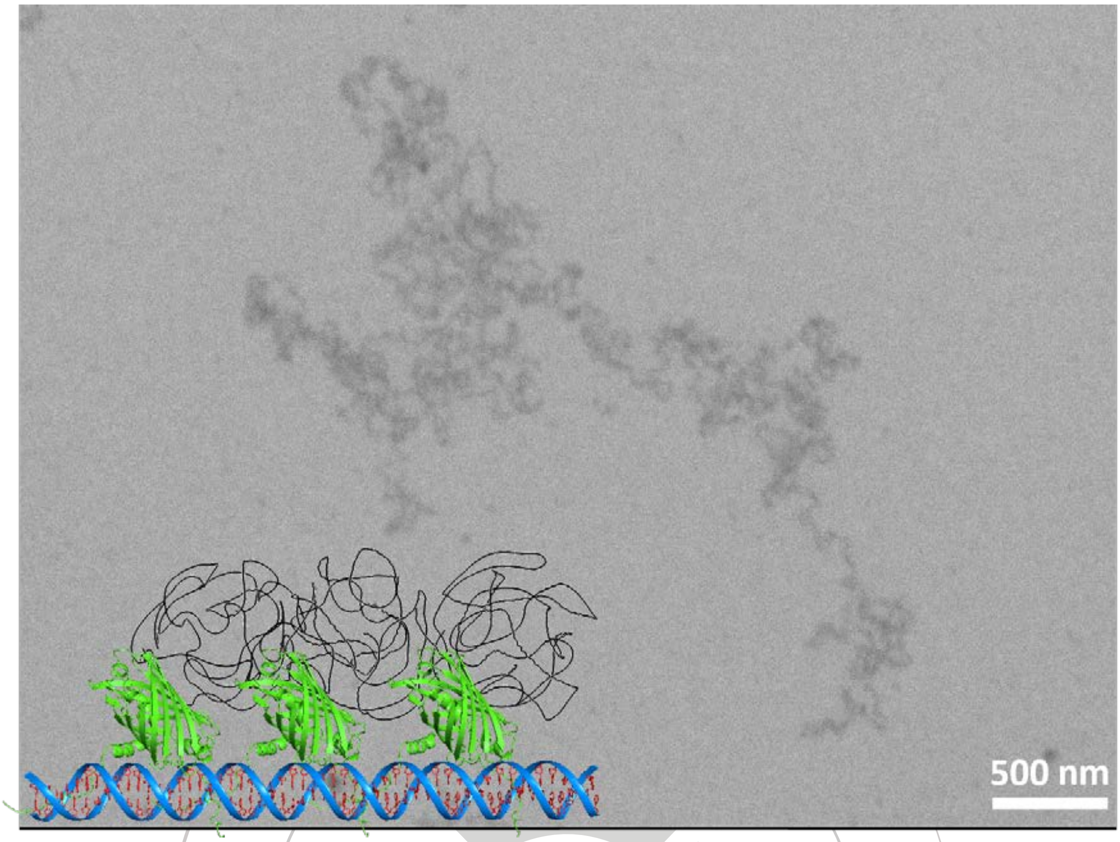
Oral Presentation : **LIFE.O-6**
Oral Presentation for Young Scientists in Biochemistry and Chemical Biology
Room 101+102 THU 09:50
Chair: Yong Woong Jun (KAIST)

Visualizing large DNA molecules through Scanning Electron Microscopy (SEM) Using a Metal-Free Electro-Stain Composed of DNA-Binding Proteins and Synthetic Polymers

Chanyoung Noh, Kyubong Jo[1,*]

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

DNA visualization is crucial in genomic research. We have developed a novel electro-stain reagent for visualizing DNA using a scanning electron microscope (SEM). This reagent is created by combining DNA-binding proteins with synthetic polymers, which improves the visibility of DNA strands, which are typically 2 nm thick, when viewed under SEM. Unlike conventional staining reagents for electron microscopy that rely on heavy metals, our method utilizes proteins and polymers to stain DNA, resulting in dark lines when viewed under SEM. The resulting images show a thickness ranging from 15.0±4.0 nm. As SEM serves as the primary platform, it seamlessly integrates with various chemically treated surfaces and microfluidic devices. Our technique enables high-resolution imaging of different DNA configurations, including linear, circular, single-stranded, and double-stranded, as well as various DNA structures, ranging from genomic and mitochondrial DNA to chromatin and chromosomes. Additionally, quantum dots were successfully visualized as bright labels specifically incorporated into the polymer-stained DNA molecules. In summary, SEM DNA imaging using this innovative electro-staining technique provides electron microscope resolution with the convenience of optical microscopy.


500 nm

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 101+102 THU 10:00

Chair: Yong Woong Jun (KAIST)

Programming heteromeric protein self-assembly with interchangeability and reversibility

Soyeun Son, Woon Ju Song*

Department of Chemistry, Seoul National University, Korea

Protein design allows for the exploration of protein-protein interfaces through diverse chemical interactions. However, in many cases, protein self-assembly relies on a single protein as a building block, limiting the chemical diversity of designed structures and functions. Heterooligomers offer a broader range of structural and functional diversity, yet their utility could be enhanced by enabling interchangeable protein components. This presentation highlights our recent design strategy for creating diverse protein heterooligomers in an easily applicable and exchangeable manner, without extensive sequence optimizations. Instead, we designed a bifunctional linker containing an enzyme inhibitor and maleimide, which resulted in four distinct two-component heterooligomers with adjustable size and assembly kinetics through the introduction of metal chelators, acidic buffer components, and reducing agents. Our design strategy facilitates interchangeability between the linker and protein components, expanding the potential of protein-assembled architectures and their applications as functional biomaterials.

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

Oral Presentation for Young Scientists in Biochemistry and Chemical Biology

Room 101+102 THU 10:10

Chair: Yong Woong Jun (KAIST)

Capillary Force Driven Microfluidic Device for Analysis of Large Single-Molecule DNA

Taesoo Kim, Kyubong Jo[*]

Department of Chemistry, Sogang University, Korea

Rapid advancements in microfluidics are propelled by its extensive applications in life sciences and biomedical engineering. A key challenge within microfluidics is the precise control and manipulation of fluids in microscale channels. Addressing this challenge, capillary force-driven flows offer a promising solution, obviating the need for external power sources. These capillary-driven flows are particularly advantageous for the consistent and reliable analysis of single-molecule DNA when integrated with a fluorescence microscope, offering a straightforward yet potent method. In this study, we have developed multiple microfluidic devices utilizing capillary force to enhance the deposition of DNA molecules onto positively charged glass surfaces from sample solutions. Optimization efforts focused on outlet reservoir capacity, surface charge density, and microchannel dimensions. These refinements enabled us to maximize DNA elongation and deposition, achieving a detection limit of 0.48 fg/μL, equivalent to 64 molecules of 7.25 kbp DNA in 1 μL, distinguishable by DNA length. The developed device serves as an ultra-sensitive platform for quantitative DNA analysis and facilitates rapid, accurate point-of-care testing with minimal detection limits. In summary, our findings underscore the potential of capillary force-driven microfluidics for reproducible and efficient fluid manipulation within microscale channels.

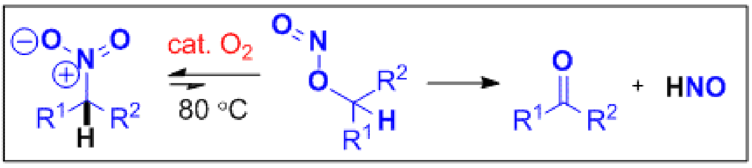
Award Lecture in Division : **ORGN.O-8**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 17:10
Chair: Jun Hee Lee (Dongguk University)

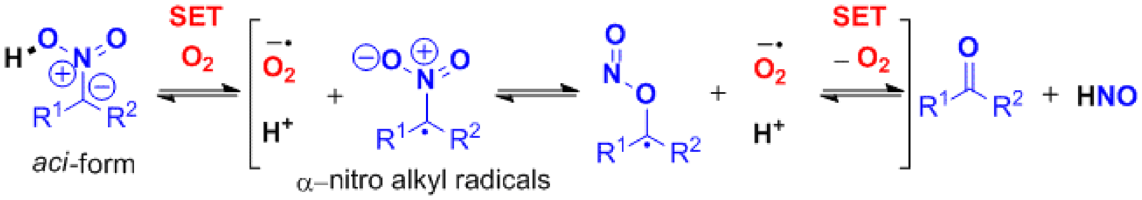
Development of Aerobic Nitro-Nitrite Isomerization Strategy as a Versatile Synthetic Tool

Kyungsoo Oh

College of Pharmacy, Chung-Ang University, United States

Nitroalkanes are high-energy materials utilized as fuels and fuel additives with favorable bond scission energetics. While the theoretical and experimental studies for the past few decades have intensified the debate on the true nature of nitroalkane decomposition pathways, the overarching theory regarding the N-C bond cleavage in nitroalkanes is based on the nitro-nitrite isomerization. Nevertheless, the debate on the nature of nitro-nitrite isomerization of nitroalkanes remains unresolved despite the extensive high-level computational modelings.The synthetic versatility of nitroalkanes stems from the ready tautomeriztion of nitro-form to *aci*-form, leading to the formation of nucleophilic nitronates under basic conditions. The utilization of nitroalkanes readily expands to the preparation of highly substituted saturated and unsaturated hydrocarbons, amines as well as carboxylic acid derivatives. Given the importance of nitroalkanes as versatile synthetic building blocks, we became interested in the decomposition pathways of nitroalkanes. In contrast to the well-established chemistry of nitronate anions, the related alpha-nitro alkyl radical species have not been recognized as a viable intermediate species. In this presentation, we will discuss various decomposition pathways of nitroalkanes using either organocatalysts or aerobic oxidation protocols. Also, the aerobic decomposition pathway of nitroalkanes will be substantiated through the single electron transfer process between the *aci*-form of nitroalkanes and molecular oxygen to give the alpha-nitro alkyl radical and superoxide radical species. The synthetic utilization of nitroalkanes as a nitrosyl species via isomerized alkylnitrites will be also discussed in the N-nitrosation of amines.


cat. O₂
80 °C
+ HNO


SET
O₂
aci-form
H⁺
+
α–nitro alkyl radicals
+
H⁺
SET
– O₂
+ HNO

Oral Presentation : **ORGN.O-1**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 15:40
Chair: Hyung Min Chi (POSTECH)

Organosuperacid Catalysis for the Synthesis of Pharmaceuticals

Woo hee Kim, Han yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

α-Secondary alkyl amines are structural scaffold frequently encountered in a wide variety of natural products and pharmaceuticals. To synthetically approach such a privileged moiety incorporated complex molecule, a protected amine strategy is considered a highly useful process. In particular, *N*-benzyloxycarbonyl (Cbz) compound is one of the most widely utilized precursors in amine chemistry. However, a direct catalytic approach toward alkyl Cbz-amine is quite rare owing to the low reactivity of carbamate. Here, we demonstrate a pinacolborane-assisted organic superacid catalyzed direct access to Cbz-protected α-secondary alkyl amines from general ketones as the starting material. Due to the highly chemoselective and robust catalytic system, a variety of substrate scopes including drug precursor scaffolds in preparative scalability (up to >99% yield) incorporating practical pharmaceutical syntheses (pyrrolidine heterocycle, Isometheptene, and Mexiletine) were achieved. Experimental, analytical, and computational studies support the pinacolborane-assisted Brønsted acid catalytic system, which efficiently facilitates the chemoselective reductive amination process. The obtained alkyl *N*-Cbz amines were observed to possess strong cytotoxicities from in vitro bioactivity evaluations, indicating their potential as promising candidates for new anticancer drug discovery.

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Oral Presentation : **ORGN.O-2**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 15:52
Chair: Hyung Min Chi (POSTECH)

A Polydiacetylene (PDA)-based Colorimetric Sensor for Detecting Cyanide Anions and Its Application to Paper Devices

Seongman Lee, Songyi Lee[1,*]

BB21+ Program, Department of Chemistry, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

In this study, we reported a polydiacetylenes-based colorimetric sensor (PDA-BMN) for cyanide anion detection and its application to a paper device. 2-Benzylidenemalononitrile was used as the acceptor for cyanide anions, reacting with cyanide anions to generate PDA-BMN-CN, resulting in the conformational transition of the conjugated backbone. An obvious color change from the blue phase to the orange phase between PDA-BMN and PDA-BMN-CN is clearly visible to the naked eye. PDA-BMN was highly selective for cyanide anions over other anions. The interaction between PCDA-BMN and cyanide anions was confirmed by Raman spectroscopy, Field Emission Scanning Electron Microscopes (FE-SEM), and Proton nuclear magnetic resonance (1H NMR). Finally, the color change observed in PDA-BMN as a response to cyanide anions was effectively demonstrated by integrating it into pressed lateral flow assay strips. This study introduces an innovative and promising approach for enhancing the capabilities of chemosensors in detecting cyanide anions.

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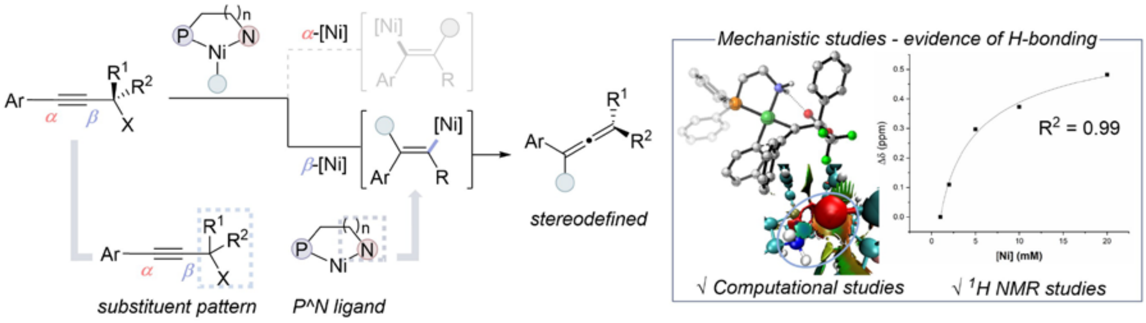
Oral Presentation : **ORGN.O-3**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 16:04
Chair: Hyung Min Chi (POSTECH)

Overriding Conventional Regioselectivity in Arylnickelation of Alkynes: Dual-controlled Stereodefined Conversion of Tertiary Acetates to Tetrasubstituted Allenes

Seoyeon Kim, Eun Jin Cho[1,*]

Chemistry, Chung-Ang University, Korea
[1]*Department of Chemistry, Chung-Ang University, Korea*

Ni-Catalyzed reactions of arylated alkynes through β-nickelation poses a significant challenge due to the formation of more stable α-[Ni]-alkenyl intermediates. In this study, we have successfully developed a Ni-catalytic system that overcomes this challenge and enables regioselective β-nickelation of arylated propargylic substrates in a stereo-defined manner. The achievement was made possible by fine-tuning the substrate- and catalytic system through ligand modulation. The efficiency of the process was greatly influenced by subtle differences in the ligand system, allowing precise control of the bite angle and coordination length. Notably, a free amino-type P^N ligand was utilized, exhibiting enhanced reactivity through hydrogen bonding interactions with the substrate. The stereo-defined nature of this transformation was confirmed through reactions with chiral substrates, demonstrating the precise control over the stereochemistry of the products.


P
Ni
N
n
α-[Ni]
[Ni]
Ar
R
Ar
α
β
R1
R2
X
β-[Ni]
[Ni]
Ar
R
Ar
R1
R2
stereodefined
Ar
α
β
R1
R2
X
substituent pattern
P
Ni
N
n
P^N ligand
Mechanistic studies - evidence of H-bonding
Δδ (ppm)
[Ni] (mM)
R2 = 0.99
√ Computational studies
√ 1H NMR studies

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 16:16

Chair: Hyung Min Chi (POSTECH)

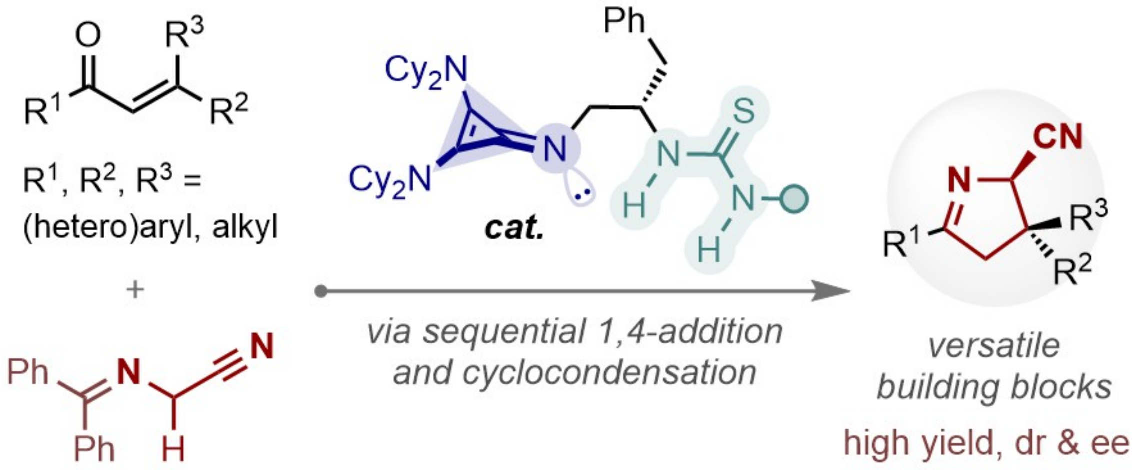
Enantio- and Diastereoselective Variations on α-Iminonitriles: Harnessing Chiral Cyclopropenimine-Thiourea Organocatalysts

<u>Hoo seung Lee</u>, Sarah Yunmi Lee[1,*]

Chemistry, Yonsei University, Korea

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

Chiral 1-pyrrolines containing a nitrile motif serve as crucial structural scaffolds in biologically active molecules and exhibit diversity as building blocks, owing to their valuable functional groups; however, the asymmetric synthesis of such compounds remains largely unexplored. Herein, we present an enantio- and diastereoselective method for the synthesis of α-chiral nitrile-containing 1-pyrroline derivatives bearing vicinal stereocenters through the design and introduction of chiral cyclopropenimine-based bifunctional catalysts featuring a thiourea moiety. This synthesis entails a highly stereoselective conjugate addition of α-iminonitriles to a wide array of enones, followed by cyclocondensation, thereby affording a series of cyanopyrroline derivatives, some of which contain all-carbon quaternary centers. Moreover, we demonstrate the synthetic utility of this strategy by per-forming a gram-scale reaction with 1% catalyst loading, along with a variety of chemoselective transformations of the product, including the synthesis of a vildagliptin analogue. Finally, we showcase the selective synthesis of all four stereoisomers of the cyanopyrroline products through trans-to-cis isomerization, highlighting the versatility of our approach.


R1, R2, R3 =
(hetero)aryl, alkyl
+
cat.
via sequential 1,4-addition
and cyclocondensation
versatile
building blocks
high yield, dr & ee

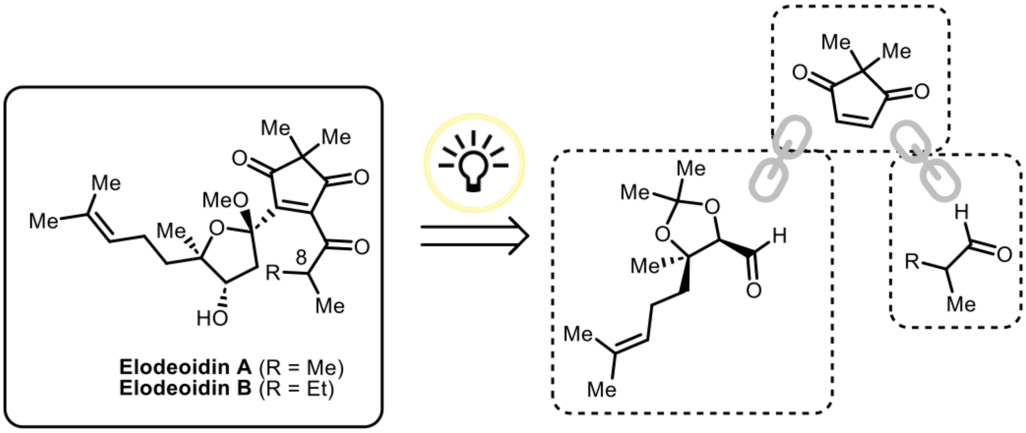
Oral Presentation : **ORGN.O-5**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 16:28
Chair: Hyung Min Chi (POSTECH)

Total Syntheses of Elodeoidins A and B Enabled by Photochemical Transformations

Chungwoo Lee, Sunkyu Han*

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

Elodeoidins A and B have been isolated by the Luo and the Kong group in 2020 from the herb of *Hypericum elodeoides*. Structurally, it possesses a unique five-membered β-diketone unit with an exocyclic carbonyl group presumably derived from an α-ketol rearrangement and this feature was not observed in other acylphloroglucinol meroterpenoids. For elodeoidin B, the absolute stereochemistry of C8 was not reported and we are aiming to elucidate its complete structure via total synthesis. In this presentation, our current research progress on the total synthesis of elodeoidin A and B will be presented. Our synthetic route fully utilizes the light-mediated transformation, a ‘hot issue’ in 21st century among the synthetic community. The main key step, formation of C2–C3 bond, was achieved via photocatalyzed cross dehydrogenative coupling which was recently developed in our laboratory.



Elodeoidin A (R = Me)
Elodeoidin B (R = Et)

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Oral Presentation : **ORGN.O-6**
Oral Presentations for Young Scholars in Organic Division
Room 304+305+306 THU 16:40
Chair: Hyung Min Chi (POSTECH)

C-C bond cleavage for the synthesis of isocyanates and their applicaion in the preparation of unsymmetrical carbonyl compounds

Seo Yeon Kim, Hee Nam Lim[1,*]

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

Despite considerable progress in the synthesis of unsymmetric carbonyl compounds using different carbonylation reagents, the establishment of dependable and eco-friendly synthetic procedures remains a challenge. In our research, we have identified methyl pyruvate oxime as a viable and safe source of carbonyl, facilitating the synthesis of a wide range of carbonyl compounds via isocyanates as key intermediates. Our investigation primarily targets nitrogen-containing carbonyl compounds, crucial constituents in pharmaceuticals, pesticides, and various functional materials. Through mild one-pot conditions, we have achieved the efficient production of diverse unsymmetrical carbonyl compounds.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentations for Young Scholars in Organic Division

Room 304+305+306 THU 16:52

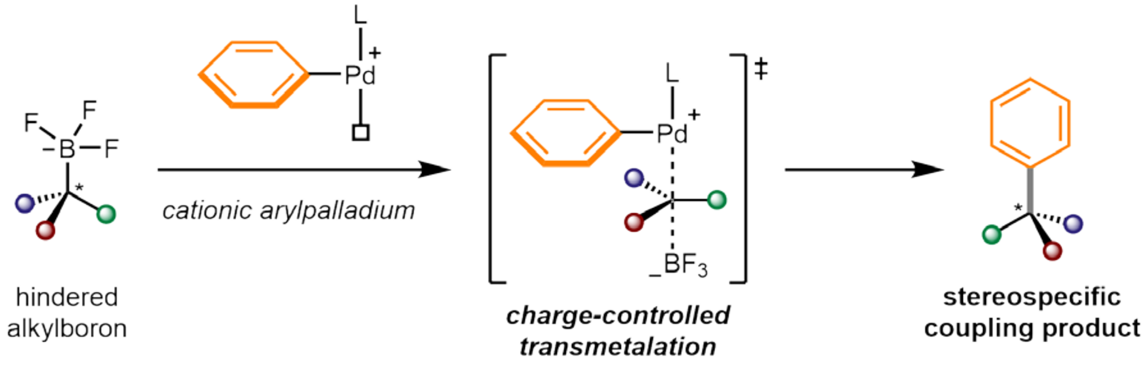
Chair: Hyung Min Chi (POSTECH)

Stereospecific Coupling Reactions of Chiral Alkylboron Compounds via Charge-Controlled Transmetalation

Won Seok Ham

Department of Chemistry, College of Natural Sciences, Seoul National University, Korea

Stereospecific functionalization of enantioenriched small molecules represents an underdeveloped, yet straightforward approach for the generation of new stereogenic centers. Chiral alkylboron derivatives are desirable substrates for stereospecific reactions due to their chemical and configurational stability, but the high covalency of the carbon–boron bonds at the stereogenic centers of those compounds compromises their reactivity in transition-metal-catalyzed cross-coupling reactions. To date, a general stereospecific reaction manifold applicable to a wide variety of alkylboron compounds has yet to be established. Here we present a solution to this problem based on an underexplored chirality-transfer mechanism. We demonstrate that a catalytically generated cationic arylpalladium complex binds with alkylboron compounds and elicits stereospecific transmetalation, consequently affording chiral alkylarene products. Our reaction is capable of functionalizing carbon–boron bonds with high steric hindrance that are otherwise difficult to activate. We provide a fundamental analysis of the charge-controlled transmetalation, which we anticipate should aid in the design of other useful stereospecific transformations.


hindered alkylboron
cationic arylpalladium
charge-controlled transmetalation
stereospecific coupling product

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 09:00

Chair: Seong Jun Park (KRICT)

Development of new target protein small molecules as a novel class of H_2O_2 scavenger for treatment of Alzheimer's Disease

Elijah Lee, Ki Duk Park[*]

Center for Brain Disorders, Korea Institute of Science and Technology, Korea

Alzheimer's disease (AD) is the most common form of dementia and is a progressive neurodegenerative disease characterized by memory loss. In the AD brain, reactive oxygen species (ROS) levels are significantly higher than that of healthy aging brain. Hydrogen peroxide (H_2O_2) is a representative ROS that causes oxidative stress and is a product of many different metabolic pathways in AD[1]. We recently investigated the mechanism of action of the drug HTPEB (AAD-2004), which is effective in scavenging H_2O_2 in neurodegenerative disease mouse model. In this study, we aim to optimize the efficacy and drug-like properties of HTPEB to develop a novel H_2O_2 target candidate for treatment of AD. We synthesized a series of novel compounds and evaluated the H_2O_2 scavenging activity using an optimized in vitro assay system. Among them, KDS12025 exhibited three times the efficacy of HTPEB (EC_{50}: 0.0449 μM to 0.1551 μM, respectively) and also showed favorable microsomal stability (57.6% in human during 30 min to

Oral Presentation : **MEDI.O-2**
Oral Presentation of Young Medicinal Chemists
Room 301+302 THU 09:13
Chair: Seong Jun Park (KRICT)

Discovery of novel YAP-TEAD interaction inhibitors for colorectal cancer treatment

On-Yu Kang, Jiyoung Hyun, Seong Jun Park, Hwan Jung Lim[*]

Data Convergence Drug Research Center, Korea Research Institute of Chemical Technology, Korea

The Hippo pathway is known to have tumor-suppressive role, and dysregulation of the Hippo signaling pathway result in tumorigenesis and overgrowth of tumor. Although most promising druggable target of the Hippo pathway is to inhibit binding YAP, a transcriptional co-activator, and TEADs, transcriptional factor in nucleus, drug candidates selectively targeting YAP-TEAD are still lacking. In this study, we identified drug-like hit compound screened from integrated 3D database, based on structural interface between YAP-TEADs. We synthesized lead compounds that showed solid structure-activity-relationship (SAR) and promising anti-cancer activities in animal models with almost no side-effects. Selective binding of an inhibitor with TEAD proteins was confirmed through various biochemical assays. We suggest that our compounds had a potential to be investigated as a drug candidate targeting YAP-TEAD binding for cancer treatment.

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 09:26

Chair: Seong Jun Park (KRICT)

Development of a novel nano-reactor assembly with 8-(N-phenylhexanamido) naphthalene-1-sulfonate, HBF4 and Fe(BF4)2, and its application to the amination of alcohol

Waqar Ahmed

Bionano Chemistry Lab (BNCL), Department of Bionano Engineering, Korea

AbstractDiverse artificial vesicles have been employed for many biomedical applications, such as drug carriers, bioreactors and gene delivery. These vesicular assemblies have not been fully studied for development of organic reactions in water, although their micellar counterparts have enormously been used for the same purpose as a green alternative system. We introduce a vesicle-like nano-reactor assemblies formed by a novel amphiphilic catalyst (8-(N-phenylhexanamido)naphthalene-1-sulfonate (Cat-3)), HBF4 and Fe(BF4)2 in water and their use as nano-reactors for development of dehydrative amination of alcohols in aqueous solution. These assemblies showed a significantly enhanced performance than the micellar catalysts, such as sodium dodecyl sulfate (SDS), sodium dodecylbenzene sulfonate (SDBS), and Brij-35 for the dehydrative amination of various alcohols. The dehydrative amination reaction utilizing Cat-3-HBF4-Fe(BF4)2-based assemblies in water was favorable owing to its efficient and environmentally-friendly set-up, easily available starting materials and non-toxic catalysts. The present method was also applied as a key step for the gram-scale total synthesis of the FDA-approved drug, naftifine. The assemblies were characterized through dynamic light scattering (DLS), ζ-potential, transmission electron microscopy (TEM) and confocal microscopy (CLM).

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 09:39

Chair: Seong Jun Park (KRICT)

Discovery of Heterocyclic Structure-Based Novel P2X3 Receptor Antagonists

Ga-Ram Kim, Yong-Chul Kim*

School of Life Sciences, Gwangju Institute of Science and Technology, Korea

P2X3 receptor, an ATP ligand-gated cation channel predominantly expressed in C- and Aδ- primary afferent nerves, has been reported as the drug target for various neurological diseases such as neuropathic pain and chronic cough. Aiming to develop novel and selective P2X3R antagonists, tetrazolopyrimidine-based hit compound was optimized through structure−activity relationship studies with modifications at the tetrazole core skeleton as well as side chain substituents. The finally optimized compound, with cyclopropane substituted triazolopyrimidine core structure, showed potent P2X3R antagonistic activity with an IC50 value of 54.9 nM with 20-fold selectivity vs P2X2/3R, which is responsible for the taste-loss side effect and low antagonistic activities at other P2XR subtypes. An in-vivo study in the spinal nerve ligation neuropathic pain rat model showed an antiallodynic effect in a dose-dependent manner.

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 09:52

Chair: Seong Jun Park (KRICT)

Exploring Novel Ligands for the 5-HT$_7$ Receptor: A Computer-Aided Drug Discovery Approach for Autism Spectrum Disorder Treatment

Haeun Lee, Gyo chang Keum*, Hyunah Choo*, Byungsun Jeon*

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

The 5-HT$_7$ (5-hydroxytryptamine, serotonin) receptor is a member of G-protein coupled receptor (GPCR) and is associated with various physiological processes in the central nervous system (CNS). Studies for the importance of serotonergic system in the early developmental stage and recent data lead 5-HT$_7$R to become a promising therapeutic target for autism spectrum disorder (ASD), a complex neurodevelopmental disorder with repetitive behavior and impaired social interaction. In this study, we carried out a computer-aided drug discovery (CADD) framework with a 5-HT$_7$ homology model to develop novel ligands. Using the ZINC and Chemdiv databases, we employed CDOCKER and LibDock calculation methods to predict the non-bond covalent interaction between a ligand and the receptor. The 54 compounds selected through the virtual screening were subsequently evaluated *in vitro*. Luminescent-based studies of the GPCR signaling pathway aided in defining the properties of the ligand, such as whether it acts as an agonist or antagonist. None of the compounds act as agonists over the signaling pathways such as the G$_s$, β-arrestin, and G$_{12}$ signaling. Remarkably, our rigorous screening protocols have led to the discovery of small molecules capable of blocking the G$_{12}$ downstream signaling cascades via 5-HT$_7$R without interfering others. We further evaluated the effects of compounds on Shank 3 Tg mice, resulting in an increase in repetitive behavior. Our findings clearly indicate that the development of an agonist for G$_{12}$ signaling is crucial, and 5-HT$_7$R appears to be a promising therapeutic target for ASD drug development.

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 10:05

Chair: Seong Jun Park (KRICT)

Catalyzing Breakthroughs: The Next Wave of Rapid and Efficient Drug Discovery

Jiwoong Lim, Kenneth H. Pearce[*]

Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, United States

Traditional drug discovery, heavily reliant on small molecule therapeutics and structure-activity relationship (SAR) studies, often faces the challenge of time-consuming synthesis and individual compound testing. While high-throughput screening techniques and virtual screening based on pharmacophore studies have expedited the hit compound identification process, they still have limitations, particularly in addressing 'undruggable' targets.Leveraging advanced display technologies for peptide drug development offers a promising solution. By integrating biomolecular display systems with next-generation sequencing, we can rapidly and efficiently identify peptide drug candidates with high affinity, selectivity, and low toxicity for previously undruggable targets. This presentation will explore various display technologies, including mRNA and Phage display, and discuss their practical application in the early stages of drug discovery, mainly focusing on oncological targets. Furthermore, focused DNA-encoded library studies will be introduced to develop drug-like peptidomimetics, capturing the best features of small molecules and peptides.

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 10:18

Chair: Seong Jun Park (KRICT)

Design and synthesis of selective JAK1 Inhibitors for the treatment of autoimmune diseases

Santosh shivanand Raikar, Pilho Kim[1,*]

Medicinal chemistry, University of Science & Technology, India

[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Janus kinase 1 (JAK1) inhibitors have emerged as a promising class of drug target for the treatment of autoimmune diseases. Autoimmune and inflammatory conditions are widespread and come in many forms, capable of impacting any part of the body. Thus, JAK inhibitors are essential for the treatment of autoimmune diseases, offering significant benefits to patients with conditions, such as rheumatoid arthritis, ulcerative colitis, and psoriasis. However, concerns over the safety and selectivity of these drugs have been raised. Several JAK1 inhibitors have been developed and are currently in clinical trials for the treatment of autoimmune diseases. Tofacitinib and baricitinib have been approved by the US FDA for the treatment of rheumatoid arthritis and atopic dermatitis, respectively. While non-selective JAK inhibitors could lead to off-target effects and potential toxicities, selective inhibitors could offer greater specificity and reduce side effects. Filgotinib, a promising selective JAK1 inhibitor, has shown encouraging results in early clinical trials and may offer more safe and effective alternative to the regimens including JAK inhibitors. To discover JAK1-selective inhibitors, novel compounds have been designed derived from filgotinib. Optimization processes, biological activities, ADME/Tox profiles will be presented. Finally, in vivo efficacy studies of selected compounds using a collagen-induced arthritis (CIA) model will be discussed.

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 10:31

Chair: Seong Jun Park (KRICT)

Structure-based drug design approach and synthesis for a new class of nucleoside A_{2A} adenosine receptor antagonist as promising immune-oncology agents

Gibae Kim

College of Pharmacy, Seoul National University, Korea

In this study, we focused on the A_{2A} adenosine receptor (A_{2A}AR), a key subtype within the adenosine receptors, as a crucial target in the development of immune-oncology therapies. Previous approaches to develop A_{2A}AR antagonists have predominantly involved the use of modified purines or related heterocyclic structures, reflecting their natural affinity to the adenosine-based endogenous ligand. A common strategy has been to eliminate the ribose group to transition the compound's function from an agonist to an antagonist, highlighting the pivotal role of the ribose-induced interaction in activating the receptor. Our research successfully developed a nucleoside-based antagonist for A_{2A}AR through structure-based drug design approach. We synthesized a series of 22 different molecules following an extensive structure-activity relationship (SAR) analysis, employing Vorbrüggen glycosylation and selective palladium-catalyzed cross-coupling reactions as key steps. The lead compound emerged with a high affinity for A_{2A}AR, exhibiting a K_i value of 7.7 nM and It completely inhibited cAMP production via A_{2A}AR signaling. Additionally, this compound was evaluated for its anti-cancer effect in vivo, where it showed a synergistic effect in combination with a mAb immune checkpoint inhibitor. Our findings introduce a new class of nucleoside-based A_{2A}AR antagonists, identified through SAR and structural analysis, with potent in vivo anti-proliferative effect, offering valuable insights into receptor activation mechanisms and potential therapeutic applications in immune-oncology.

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

Oral Presentation of Young Medicinal Chemists

Room 301+302 THU 10:44

Chair: Seong Jun Park (KRICT)

Macrocyclic compounds as GLS Inhibitor for anticancer agents 2

Rajath Cyriac, YeongJu Kwon[1], Kwangho Lee[2,*]

Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, University of Science & Technology, Korea

[1]College of Pharmacy, Chungnam National University, Korea Research Institute of Chemical Technology, Korea

[2]University of Science & Technology, Korea Research Institute of Chemical Technology, Korea

Glutamine-addicted cancer metabolism is recently recognized as novel cancer target especially for KRAS and KEAP1 co-occurring mutations. Selective glutaminase1 (GLS) inhibition was reported using BPTES which has novel mode of allosteric inhibition. However, BPTES is a highly hydrophobic and symmetric molecule with very poor solubility which results in suboptimal pharmacokinetic parameters and hinders its further development. To identify more drug-like GLS inhibitors via systematic structure−activity relationship (SAR) analysis of BPTES analogs, we have disclosed our novel reverse-amide macrocycles for GLS inhibition with conclusive SAR analysis on the core, core linker, and wing linker, respectively. As a part of follow-up study, we present amide macrocycles for GLS inhibition with unique SAR analysis. Selected molecules resulted in reduction in intracellular glutamate levels in LR (LDK378-resistant) cells which is consistent to A549 and H460 cells viability result.

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 09:00

Chair: Gwangwoo Kim (Chungbuk National University)

Dynamic Optical Properties of Anisotropic Gold/Iron Oxide Nanohybrids

Hyojung Kang, So-Jung Park[1,*]

Ewha Womans University, Korea

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

The ability to control the alignment of anisotropic plasmonic nanoparticles enables selective excitation of desired plasmonic modes. Here, we developed a new strategy to synthesize anisotropic gold/iron oxide nanoparticles, where the intrinsic superparamagnetic nature of the outer iron oxide shell allows rapid, reversible, and remotely controlled alignment of anisotropic plasmonic nanoparticles. This synthesis method can be applied to anisotropic nanoparticles with various sizes, aspect ratios, and shapes, illustrating the generality of this strategy. Anisotropic nanoparticles aligned along a magnetic field exhibit distinct optical properties depending on their arrangement. Linearly aligned anisotropic nanoparticles exhibit a range of transmitted light colors depending on the polarization angle. This offers the possibility of encoding information with different colors that are only visible under polarized light. Additionally, helically aligned nanoparticles form chiral nanostructures with noticeably high g-factors (>0.2 in the visible region). This research contributes a pathway to tunable plasmonic/magnetic nanoparticles, opening new avenues for advancements in materials science, optics, and information technology.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 09:15

Chair: Gwangwoo Kim (Chungbuk National University)

Exsolution-assisted immobilization of single atom catalysts to optimize their electrocatalytic activity

Dong Hoon Sun, Xiaoyan Jin[1], Seong-Ju Hwang[*]

Department of Materials Science and Engineering, Yonsei University, Korea
[1]*Department of Applied Chemistry, University of Seoul, Korea*

Single atom catalysts have evoked tremendous research activity because of their high catalytic activity for various reactions. However, the structural instability of these atomic species caused by large surface energy has detrimental effect on their electrocatalyst performances. As an effective method to overcome this drawback of single atom catalysts, we develop a phosphidation-induced exsolution approach to immobilize single atom catalysts in conductive metal phosphide matrix. The phosphidation of Ru-substituted Ni-Fe-layered double hydroxide (LDH) leads to the embedding of Ru single atom catalysts as well as to the phase transition from Ni-Fe-LDH to conducive nickel iron phosphide. The exsolved Ru single atom catalysts show excellent electrocatalytic performance and high durability as hydrogen evolution reaction catalysts, which are much superior to those of Ru-substituted Ni-Fe-LDH and Ru-deposited nickel iron phosphides. The impact of phosphidation-driven exsolution approach can be attributed to the strong electronic coupling between Ru metal atoms and conductive metal phosphide substrate.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 09:30

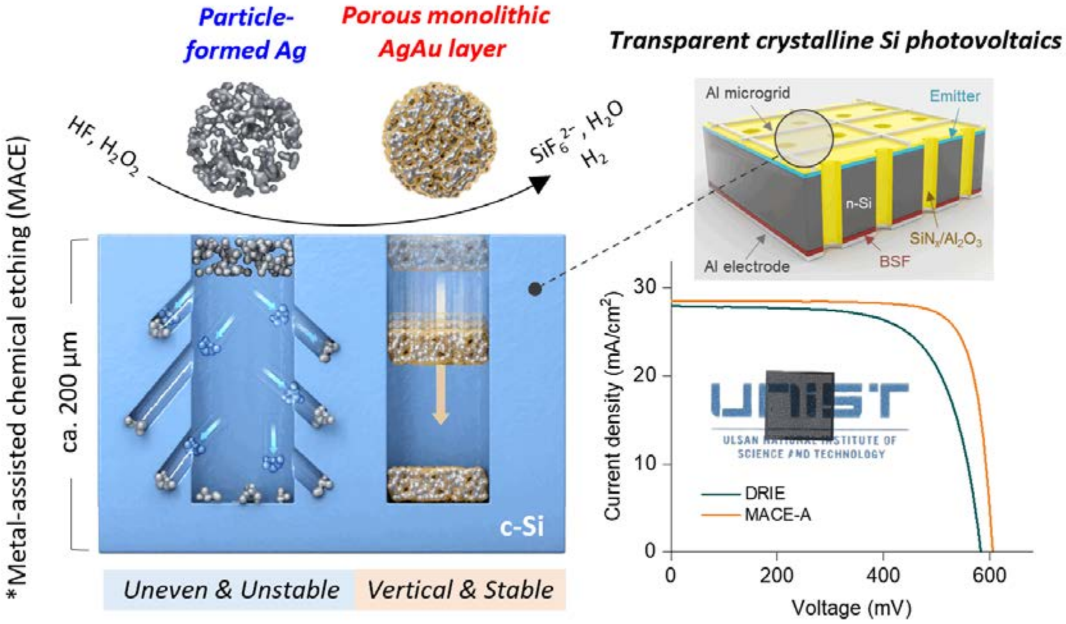
Chair: Gwangwoo Kim (Chungbuk National University)

Deep metal-assisted chemical etching using a porous monolithic AgAu layer to develop neutral-colored transparent silicon photovoltaics

HyeonOh Shin, Tae-Hyuk Kwon*

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

Neutral-colored transparent crystalline silicon photovoltaics (c-Si TPV) was reported as remarkable building-integrated photovoltaics (BIPV) due to its high efficiency with excellent transmittance. Deep reactive ion etching (DRIE) is required to fabricate this photovoltaics where the microhole-shaped light transmission windows were placed on bare crystalline silicon (c-Si, ca. 200 μm thickness) to transmit all visible wavelengths, which causes both high fabrication cost and the plasma damage on Si surface. A prominent replaceable method is metal-assisted chemical etching (MACE) which occurs through the redox reaction at the Si/metal catalyst/etchant solution interfaces because it features simplicity, versatility, and cost-effectiveness. However, the metal catalysts that grow via electroless deposition are deposited as particle-form, which act individually during MACE and induce the uneven MACE, thus yielding a lot of defects on the resultant Si.Here, we report deep MACE using a porous monolithic AgAu layer on c-Si for fabricating c-Si TPV. To prevent the uneven etching of c-Si by Ag particles, the porous monolithic Ag layer is developed by introducing acetonitrile (AN) to enhance the interaction between the c-Si surface and Ag precursor. This results in cooperative motion during MACE, as confirmed by microscopic observation, surface area measurement, and computational simulations. The durability of this Ag catalyst can be further improved by passivation with Au via galvanic replacement (i.e., the porous monolithic AgAu layer), thereby preventing indiscriminate defect generation. Thus, the fabricated c-Si TPV using MACE and a porous monolithic AgAu layer exhibits high performance of 13.0% with 20% neutral-colored transparency, representing results superior to those obtained with samples fabricated by DRIE (11.5%).


Particle-formed Ag
Porous monolithic AgAu layer
Transparent crystalline Si photovoltaics
HF, H_2O_2
SiF_6^{2-}, H_2O
H_2
*Metal-assisted chemical etching (MACE)
ca. 200 μm
c-Si
Uneven & Unstable
Vertical & Stable
Al microgrid
Emitter
n-Si
SiN_x/Al_2O_3
BSF
Al electrode
Current density (mA/cm^2)
Voltage (mV)
0
10
20
30
0
200
400
600
DRIE
MACE-A
UNIST
ULSAN NATIONAL INSTITUTE OF SCIENCE AND TECHNOLOGY

Oral Presentation : **MAT.O-4**
Oral Presentation for Young Material Chemists
Room 407+408 THU 09:45
Chair: Gwangwoo Kim (Chungbuk National University)

Orientation-controlled synthesis of covalent organic framework thin film via acid catalyst-assisted chemical vapor deposition

YeLim Son, Hee Cheul Choi*

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

The facile synthesis of thin films of covalent organic frameworks (COFs) is one of the key subjects in the COF society. Although recent studies utilizing vapor phase reactions, such as chemical vapor deposition (CVD) and molecular layer deposition (MLD), have shown their potential, achieving both high crystallinity and orientation control in 2D COF thin films is still challenging. In this presentation, we report on our recent progress in the orientation-controlled synthesis of COF thin films via acid-catalyst-assisted CVD. We have achieved the preparation of large-area COF thin films with high crystallinity and a unique edge-on orientation through the template effect of an acid catalyst. Additionally, we propose a growth model for COF-LZU1 thin films, involving a p-toluenesulfonic acid (PTSA) catalyzed imine condensation reaction between 1,3,5-triformylbenzene (TFB) and p-phenylenediamine (PDA) molecules. Our findings not only introduce a novel method for orientation-controlled COF thin film synthesis but also offer valuable insights into the structure-directing role of the acid catalyst in the growth mechanism of COF thin films.

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 10:00

Chair: Gwangwoo Kim (Chungbuk National University)

High-performance n-type SnSe thermoelectrics by simultaneously engineering electronic and phonon band structures

Sejin Byun, Chung In[1,*]

Chemical and biological engineering, Seoul National University, Korea

[1] School of Chemical & Biological Engineering, Seoul National University, Korea

Thermoelectric (TE) technology enables sustainable power generation by directly converting heat into electrical energy. Consequentially, it can uniquely utilize waste heat, accounting for approximately 67% of the total energy input worldwide, to efficiently generate useable electric energy. It is a silent and vibrationless energy harvesting system, ensuring strong mechanical stability and no environmental impact without generating harmful chemicals such as greenhouse gases. With flexibility in size and structure of devices, TE modules show great promise in powering microelectronics, flexible electronics, and traditional industrial applications such as chemical plants and automobiles. Recent advancements in polycrystalline SnSe-based materials, which exhibit ultrahigh TE performance, represent a significant breakthrough in the field of thermoelectrics. Unlike p-type polycrystalline SnSe materials, however, the development of n-type counterparts is still highly challenging due to its intrinsic p-type conduction nature and lack of effective TE performance-enhancing strategies. Here, we report the new n-type TE system $Cd_x(Sn_{0.76}Pb_{0.24})_{1-x}Se_{0.98}Cl_{0.02}$ ($x = 0, 0.0025$), exhibiting record high TE figure of merit, ZT, values. The divalent Pb and Cd successfully stabilize n-type carrier in SnSe. They favorably modulate electronic and phonon band structures concurrently according to our DFT calculations. The introduced Cd creates the unique atomic-level defect structures in the SnSe matrix, thereby reducing lattice thermal conductivity, without sacrificing carrier transport. These results synergistically boost a maximum ZT to ~2.23 at 873 K and provide the new strategy to enhance TE performance of polycrystalline n-type SnSe system.

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 10:15

Chair: Gwangwoo Kim (Chungbuk National University)

Designing Ni Single Site Catalysts Mimicking the Ni SOD Enzyme for Efficient H_2O_2 Electrosynthesis

Sang Hoon Joo*, June Sung Lim

Department of Chemistry, Seoul National University, Korea

Hydrogen peroxide (H_2O_2), a colorless, odorless, and weak acidic oxidizing agent, is one of important commodity chemicals with a wide range of applications, from disinfectants to semiconductor etchants. The electrosynthesis of H_2O_2 via oxygen reduction (2e$^-$ ORR) has emerged a promising means of H_2O_2 production, as it allows clean, continuous, and on-site H_2O_2 production. We design a series of atomically dispersed Ni catalysts (Ni ADCs) for H_2O_2 electrosynthesis, inspired by an H_2O_2-producing metalloenzyme called nickel superoxide dismutase (Ni SOD) with cofactor structures, which comprises a distorted square planar Ni^{2+} site, phenol group in tyrosine, and amine group in cysteine. The preparative chemistry of Ni ADCs was comprehensively explored, and we found that the formation of distorted square planar $Ni^{2+}–N_x$ sites and an appropriate distortion degree are important for boosting H_2O_2 electrosynthesis activity. The optimized Ni ADC exhibited the best H_2O_2 electrosynthesis performance among the reported non-precious metal catalysts. By subjecting the optimized Ni ADC to post-synthetic heat treatments, different types of heteroatom functionality were generated. The catalyst possessing edge phenol and amine groups with distorted square planar $Ni^{2+}–N_x$ sites exhibited further enhanced catalytic activity. The KCN poisoning experiment and TOF calculation revealed a synergistic effect between the $Ni^{2+}–N_x$ sites and heteroatom functionalities.

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 10:30

Chair: Gwangwoo Kim (Chungbuk National University)

Optimizing Alkyl Chains of Non-fullerene Acceptors for Enhanced Printability in Organic Photovoltaic Modules Over 200 cm^2 Using Non-halogenated Solvent

Bomi Kim, Taeyoon Kim, Hyegyeong Hwang, Suhyun Kim, BongSoo Kim*

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

Organic solar cells (OSCs) offer sustainable energy solutions with advantages like light-weight and flexibility. The solution-processibility of organic materials enables the economical fabrication of large-area organic solar modules. However, the prevalent use of toxic halogenated solvents (e.g., chloroform, chlorobenzene, etc.) for OSC fabrication raises environmental and health concerns, highlighting the need for alternatives with low toxicity such as non-halogenated solvents (e.g., o-xylene, etc.). Moreover, a critical issue reducing the performance of OSC is the significant aggregation of non-fullerene acceptors (NFAs) causing the unfavorable film morphology during the solidification of the active layer. These problems are worse when fabricating large-area modules which take longer time to solidify active layers. In this work, we developed the NFAs as a derivative of L8-BO(EH-EH) by substituting the original alkyl chains with longer ones on pyrrole to reduce the aggregation of NFAs by increasing solubility of NFAs in o-xylene. Specifically, we replaced the 2-ethylhexyl groups on L8-BO(EH-EH) with longer ones to produce derivatives such as L8-BO(HU-HU), L8-BO(HU-DT), and L8-BO(HU-DH), which show improved solubility and film uniformity in o-xylene. These modifications lead to o-xylene-processed organic solar modules with an area of 200 cm^2 exhibiting power conversion efficiencies over 10%. Comprehensive analyses, including GIWAXS and AFM, demonstrate the effects of alkyl chain optimization on NFA aggregation and film morphology. This work emphasizes the importance precisely optimizing alkyl chains of NFA to enhance film printability and suppress severe aggregation of NFAs in the fabrication of large-area organic solar modules using non-halogenated solvents.

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

Oral Presentation for Young Material Chemists

Room 407+408 THU 10:45

Chair: Gwangwoo Kim (Chungbuk National University)

Amorphous Intermediates-Mediated Degradation of Quantum-Sized Semiconductor Nanocrystals upon Exposure to Moisture

Hyeonjong Ma, Jiwoong Yang*

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

Deciphering the degradation mechanism induced by moisture in semiconductor nanocrystals is essential for their successful application, given their higher susceptibility to moisture. Recent advancements in in-situ liquid-phase transmission electron microscopy offer the promising way for investigating degradation reactions of nanocrystals. In our presentation, we will introduce the degradation mechanism of quantum-sized semiconductor nanocrystals using the graphene double-liquid-layer cells enabling effective regulation of reaction initiation. Through the atomic-scale imaging, the degradation trajectories of CdS nanorods was investigated in detail by exploring the structure dynamics of both crystalline and non-crystalline domains during the degradation. Our findings reveal a distinct decomposition process characterized by the formation of amorphous phases, deviating from conventional metal nanocrystals etching. Notably, the degradation occurs even without electron beam, clearly supporting moisture-induced nature of the reaction. This work provides insight into previously unexplored pathways for water-induced deformation in semiconductor nanocrystals, emphasizing the crucial role of non-crystalline intermediates.

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 09:10

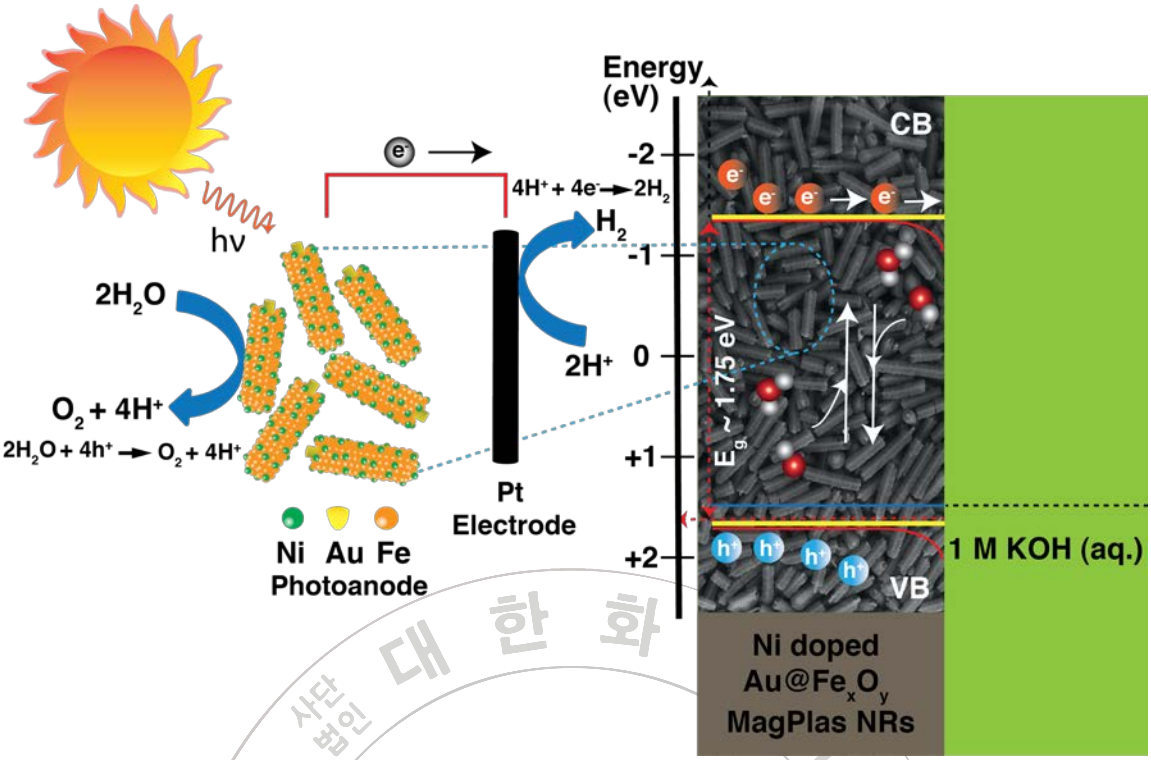
Chair: Jihyun Jang (Sogang University)

Field-driven rugged forest morphology of 1D Ni-doped Au@FexOy magnetoplasmonic nanorods for photoelectrochemical water splitting

Goddati Mahendra, **Jaebeom Lee**[1,*]

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Korea
[1]*Chemistry, Chungnam National University, Korea*

A feasible nanoscale framework of plasmonic heterogeneous materials and proper surface engineering can improve photoelectrochemical water-splitting performance owing to increased light absorption, efficient bulk carrier transport, and interfacial charge transfer. This work introduces a new magnetoplasmonic Ni-doped Au@FexOy nanorods as a novel photoanode for PEC water splitting. MagPlas Ni/Au@FexOy nanorods were synthesized by a two-step process, i.e., one-pot solvothermal synthesis of Au@FexOy, where FexOy is a hybrid of Fe2O3 and Fe3O4 and its sequential hydrothermal treatment for Ni doping. Then, a transverse magnetic field-induced assembly was adopted to decorate Ni/Au@FexOy's on FTO glass to be an artificially roughened morphologic surface called a rugged forest, which allows more light absorption. Then, to characterize its optical and surface properties, COMSOL Multiphysics simulations were carried out. The water oxidation performance of the most optimized Ni/Au@FexOy photoanode was shown as 2.73 mA cm−2 at 1.23 VRHE, where it revealed that MagPlas nanorods structure with rugged morphology provides more active sites and oxygen vacancies as the hole transfer medium, high scattered light absorption to improve the interface charge transfer performance of the photoanode. The current observation probably provides important insights into plasmonic photocatalytic hybrids and surface morphology in fabricating efficient photoanodes for PEC.


hν
2H$_2$O
O$_2$ + 4H$^+$
2H$_2$O + 4h$^+$ → O$_2$ + 4H$^+$
e$^-$ →
4H$^+$ + 4e$^-$ → 2H$_2$
H$_2$
2H$^+$
Ni Au Fe
Photoanode
Pt
Electrode
Energy
(eV)
-2
-1
0
+1
+2
CB
VB
e$^-$
h$^+$
E$_g$ ~ 1.75 eV
1 M KOH (aq.)
Ni doped
Au@Fe$_x$O$_y$
MagPlas NRs

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 09:20

Chair: Jihyun Jang (Sogang University)

Unraveling Mechanisms and Cation effects on Cu in Electrochemical Nitrate Reduction for Ammonia

<u>Minyoung Shim</u>, Hye Ryung Byon[1,*]

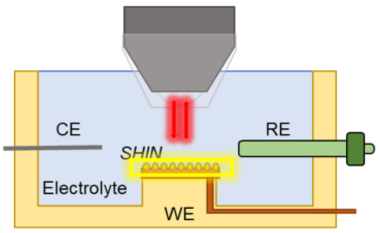
Chemistry, Korea Advanced Institute of Science and Technology, Korea

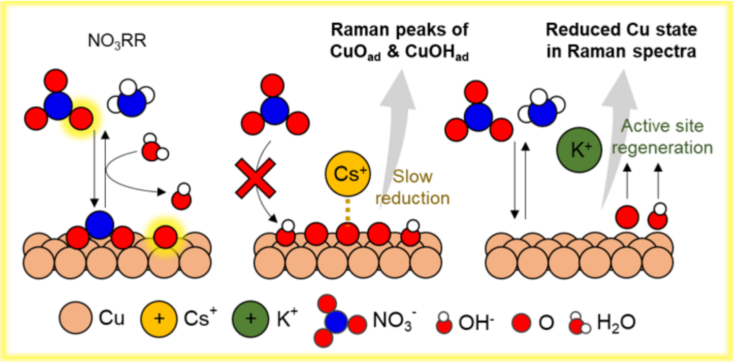
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

While the Haber-Bosch method has been widely employed to meet the industrial demand for ammonia (NH3) supply, its extensive energy requirements and CO2 emissions pose significant environmental concerns. In response to these issues, recent efforts have explored new approaches that leverage sustainable energy sources or pollutants. Notably, the nitrate anion (NO3-) is a common pollutant in aquatic ecosystems and has shown activity for electrochemical reduction to produce NH3. The fundamental understanding of the electrochemical nitrate reduction reaction (NO3RR) is an ongoing exploration, including the investigation of the effect of counter cations on NOx- adsorption and subsequent reaction processes.In this study, we utilized K+ and Cs+ ions with NO3- to investigate the product selectivity of NH3 and the underlying mechanisms. Using (100) facet-dominant copper (Cu) substrates as catalysts, cathodic linear sweep voltammetry revealed a lower overpotential for NO3− reduction in the presence of Cs+ compared to K+. However, the NO3RR was observed to be rapidly deactivated with Cs+, resulting in a low Faradaic efficiency for NH3. Operando shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) analysis unveiled the formation of CuxO and Cu(OH)2 on the Cu substrate during NO3RR in the presence of Cs+. In contast, this phenomenon was not observed with K+. Isotope analysis using N18O3- elucidated the origin of deactivation. The initial adsorption and deoxygenation of N18Ox- leaves behind 18O on the Cu substrate in the presence of Cs+, resulting in Cux18O and Cu(18OH)2, along with associated water dissociation. DFT calculations predict a thermodynamically unfavorable reduction of adsorbed O to H2O when Cs+ approaches the Cu surface,

possibly due to the water-deficient solvation shell of Cs+. I will discuss the detailed effects of Cs+ and K+ using various electrochemical and Raman analyses in this presentation.

Operando Shell-isolated nanoparticle-enhanced Raman spectroscopy





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

Oral Presentation for Young Electrochemists

Room 105+106 THU 09:30

Chair: Jihyun Jang (Sogang University)

Investigation of Electroorganic Reactions via Electroanalytical Approaches

Jaeho Shin

CO2 & Energy Research Center, Korea Research Institute of Chemical Technology, Korea

Organic electrosynthesis has drawn great attention in the recent decade to enable organic synthesis in a green, economic, and sustainable manner by replacing chemical additives with electrons. Many efforts have been made among organic chemists to electrify their chemistry and finding new reactivity of electroorganic reactions compared to conventional organic reactions in a beaker. However, such studies commonly lacked an understanding of the reaction at the electrochemical interface. In this talk, I will discuss the development of a thin-layer electroanalytical microchip (TEAM) to investigate electroorganic reactions via electroanalytical approaches.[1] It provided better resolution of voltammetry via thin-layer electrochemistry. Moreover, it enabled rapid and accurate determination of the number of electrons transferred by mechanically confining a micro-liter volume of analyte at the working electrode. Nevertheless, spectroelectrochemical analysis was possible. By applying this tool to study alkyltrifluoroborate salts, it led to a rational design of an electrochemical pathway for synthesizing carbon-heteroatom bonds via the carbocationic pathway.[2]References(1)Shin, S. J.; Kim, J. Y.; An, S.; Kim, M.; Seo, M.; Go, S. Y.; Chung, H.; Lee, M. K.; Kim, M. G.; Lee, H. G.; Chung, T. D. Revisiting Thin-Layer Electrochemistry in a Chip-Type Cell for the Study of Electro-Organic Reactions. Anal. Chem. 2022, 94 (2), 1248–1255.(2)Go, S. Y.; Chung, H.; Shin, S. J.; An, S.; Youn, J. H.; Im, T. Y.; Kim, J. Y.; Chung, T. D.; Lee, H. G. A Unified Synthetic Strategy to Introduce Heteroatoms via Electrochemical Functionalization of Alkyl Organoboron Reagents. J. Am. Chem. Soc. 2022, 144 (20), 9149–9160.

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Oral Presentation : **ELEC.O-4**
Oral Presentation for Young Electrochemists
Room 105+106 THU 09:40
Chair: Jihyun Jang (Sogang University)

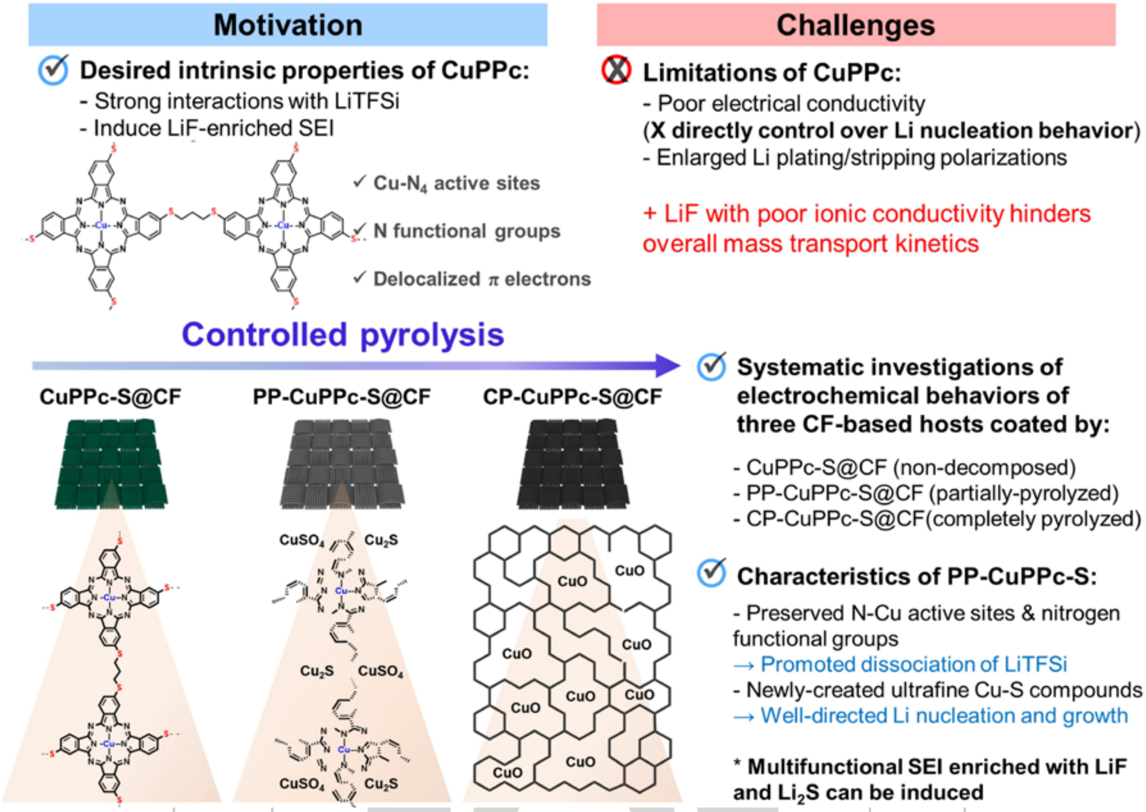
Ultra-high lithium utilization efficiency realized by partially-pyrolyzed sulfur-bridged copper polyphthalocyanines for superior cyclability of anode-free lithium metal batteries

Minjun Bae, Yuanzhe Piao[1,*]

Graduate school of convergence science and technology, Seoul National University, Korea
[1]*Graduate School of Convergence Science and Technol, Seoul National University, Korea*

Anode-free lithium metal batteries (AFLMB) can maximize the energy density by eliminating weight of active materials, conductive agents and binders. However, intrinsic challenges arising from using metallic lithium (Li) as anode, such as non-uniform Li growth, large volume changes and unstable solid-electrolyte interphase (SEI), become much more pronounced in AFLMB, significantly hindering its adoption. To circumvent these issues, an ideal current collector for AFLMB should possess followings: 1) the capability to facilitate dense and uniform Li growth, 2) the ability to induce a multifunctional SEI, 3) high lithiophilicity to lower voltage polarizations, and 4) mechanical flexibility to withstand volume changes. Herein, we propose a carbon-based three-dimensional (3D) current collector coated by partially-pyrolyzed sulfur-bridged copper polyphthalocyanines (PP-CuPPc-S@CF) as a superior AFLMB host. By intensive microscopic and spectroscopic analyses, we demonstrate that PP-CuPPc-S successfully inherited desirable redox active sites of CuPPc-S, such as N-Cu active site and N functional groups, which can promote the dissociation of LiTFSi to induce a salt-derived SEI. Simultaneously, newly-formed ultrafine Cu-S inorganic particles not only direct ultra-dense spherical Li growth, but induce ionically conductive Li_2S in the SEI. Benefiting from such synergistic effects, PP-CuPPc-S@CF achieves ultra-high Li utilization efficiency. To be specific, PP-CuPPc-S@CF with no excess Li achieved stable operation with $LiFePO_4$ (LFP, 18 mg cm-2) for 1000 cycles at 0.5C with an unprecedented capacity

retention of 81.6 %. Even when paired with 29.7 mg cm-2 of LFP, PP-CuPPc-S@CF achieved an impressive capacity retention of 49 % after 200 cycles.



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

Oral Presentation for Young Electrochemists

Room 105+106 THU 09:50

Chair: Jihyun Jang (Sogang University)

Fe doped cobalt selenide stabilizes Co state and induce dual-site mechanism for an efficient oxygen evolution reaction in AEM water electrolysis

Yo Seob Won

Energy Science, Sungkyunkwan University, Korea

Anion exchange membrane (AEM) water electrolyzers are recognized as promising solution for green hydrogen production. However, the efficiency of AEM water electrolysis comprehensively depends on the oxygen evolution electrocatalyst, which plays a critical role in determining both cell voltage and stability. In this study, we present the design and synthesis of CoFeSe2 as an efficient oxygen evolution reaction (OER) catalyst aimed at promoting a dual-site mechanism capable of effectively break the scaling relationship between intermediates (OOH* and OH*). By incorporating Fe into CoSe2, we successfully modulate the electronic structure, while maintaining the spin state of Co3+. The resulting CoFeSe2/NF catalyst exhibits outstanding OER activity, achieving overpotentials of 302 mV for the OER in 1 M KOH at a current density of 100 mA cm–2, with remarkable stability over 600 h without significant potential loss. Voltage-dependent soft X-ray absorption spectroscopy (XAS) and operando Raman spectroscopy confirm the spin state of Co3+ and surface reconstructed CoFeOOH, respectively. Furthermore, we demonstrate the partical application of the CoFeSe2 OER electrocatalyst in AEM water electrolysis by assembling an AEM device using CoFeSe2 coupled with NiMo and a sustainion membrane (1 M KOH, 80 ºC). This device requires a cell voltage of 1.81 V to reach a current density of 500 mA cm−2, maintaining stability for over 100 h. Our findings highlight the potential of CoFeSe2 as a promising catalyst for real-world applications in AEM water electrolysis.

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 10:00

Chair: Jihyun Jang (Sogang University)

[Withdrawal] Fabrication of Disposable Lactate Sensor Using $Ni(OH)_2$-Au Nanocomposite Film

Palinci nagarajan Manikandan, Kwang Pyo Kim[1,*], Jae-Joon Lee[2,*]

Dongguk University, India
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*
[2]*Department of Energy and Materials Engineering, Dongguk University, Korea*

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 10:10

Chair: Jihyun Jang (Sogang University)

Direct Growth of TiO2-IrO2 Core-Shell Catalyst onto Ti Felt for Efficient Oxygen Evolution Reaction

Jegon Lee, Bora Seo*

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

Efficient hydrogen production via water electrolysis presents a promising way to advance toward a sustainable future. In particular, proton exchange membrane water electrolysis (PEMWE) stands out as an attractive system for carbon-free hydrogen production due to its high performance, compact design, and rapid response to load fluctuations. However, the widespread implementation of PEMWE faces hurdles due to the high cost of cell stacks, primarily attributed to the use of precious metals like Ir, Ru, and Pt. To surmount this challenge, enhancing the efficiency and utilization of precious metal-based electrocatalysts is imperative. In this regard, this presentation introduces a novel method to enhance the oxygen evolution reaction (OER) efficiency of IrO2 under acidic conditions. This approach involves employing a core-shell structure featuring a Ti-based core and an IrO2 shell, and to grow the catalyst layer directly onto a Ti felt substrate. The core-shell structure offers a significant advantage in improving the mass activity of the entire catalyst layer. Moreover, the direct growth of the catalyst layer onto porous transport layer (Ti felt) ensures intimate contact and thermodynamic stability of the hetero-interface between the catalyst and substrate. As a result, the directly grown TiO2-IrO2 core-shell catalyst demonstrates superior catalytic performance for the acidic OER compared to commercial IrO2 catalysts. Furthermore, optimizing the calcination temperatures for synthesizing the IrO2 shell layer within the range of 200°C to 500°C yields the highest OER activity at 300°C, attributed to the partial formation of a highly active amorphous IrOx layer. This study proposes a promising approach for enhancing the utilization of precious metals in PEMWE applications.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 10:20

Chair: Jihyun Jang (Sogang University)

Revealing the Storage and Cycling Performances of Dual-salt Polymer Electrolytes for High-performance and Stable Li-metal Batteries

Junho Bae, Jongwoo Lim*

Division of Chemistry, Seoul National University, Korea

Polyethylene oxide (PEO)-based electrolytes are widely studied for their affordability and processability in lithium-metal batteries (LMBs). Despite significant research on lithium plating/stripping and solid electrolyte interphase (SEI) formation during cycling, the impact of lithium corrosion during aging and cycling has been unexplored. Herein, depth-profiling X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations, coupled with electrochemical analysis, unveils the intricate interplay between SEI growth, interface resistances, and their effects on LMBs during storage and cycling. Electrolytes with LiTFSI, LiBOB, and LiDFOB produced unpassivated SEIs, with anions playing no active role in SEI formation, increasing interfacial resistance and concentration gradients. In contrast, LiBF4 formed passivated SEIs, reducing interfacial resistance, thereby extending the lifespan of LMBs. Furthermore, an independent relationship was observed between the corrosion and lithium deposition. Importantly, even with uniform lithium deposition, side reactions significantly contribute to the deterioration of both electrolytes and active materials. Moving beyond conventional dual-salt electrolytes, integrating fluoroethylene carbonate (FEC) into the electrolytes enhances lithium morphology. This enhancement is particularly evident in D-LiBF4 FEC electrolytes, extending LMBs lifespan to an 10,000 hours at 0.1 mA cm^{-2}. Highlighting the crucial role of lithium corrosion, our findings offer insights for developing polymer electrolytes that boost lithium-metal battery performance.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 10:30

Chair: Jihyun Jang (Sogang University)

Tailoring Co_3O_4 Nanocubes with Noble Metal for Enhanced Electrochemical Water Oxidation

Joon Yong Park, Hyeon Beom Cho, Ki Min Nam[*]

Department of Chemistry, Pusan National University, Korea

Recently, renewable and alternative clean energy to deal with pivotal environmental problems and depletion of fossil fuels were developed. Among them, water electrolysis for H_2 production has received much attention as a feasible technology for practical application. However, the slow kinetics of the complex multi-electron transfer process at the anode side for the oxygen evolution reaction (OER) lead to deficient catalytic efficiency due to high overpotentials. Therefore, tremendous effort has been made to improve OER activity and energy conversion efficiency through the design of electrocatalysts. Although freshwater has been widely employed, there is a growing interest in seawater, which is more abundant on Earth. Seawater contains 0.5 M NaCl and exhibits high conductivity due to various ions, making it more suitable for electrolysis. In this study, we synthesized Co_3O_4 nanocubes (~150 nm) and then, performed photodeposition of Ir or/and Pd to improve electrochemical catalytic activity. Using noble metals, the prepared catalysts were subjected to the oxygen evolution reaction (OER) and chloride oxidation reaction (COR) to assess their intrinsic electrocatalytic activity and selectivity towards oxygen and active chlorine. The results of noble metal-decorated Co_3O_4 indicated the effectiveness of the metal nanoparticles in enhancing water splitting. Ir-based catalysts significantly improve OER catalytic activity, while Pd-based catalysts demonstrated excellent performance under simulated seawater conditions. Moreover, both deposited catalysts exhibited synergistic behavior under OER and CER conditions compared to other metal electrodes. These findings contribute to facilitating hydrogen generation and advancing the hydrogen economy.

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

Oral Presentation for Young Electrochemists

Room 105+106 THU 10:40

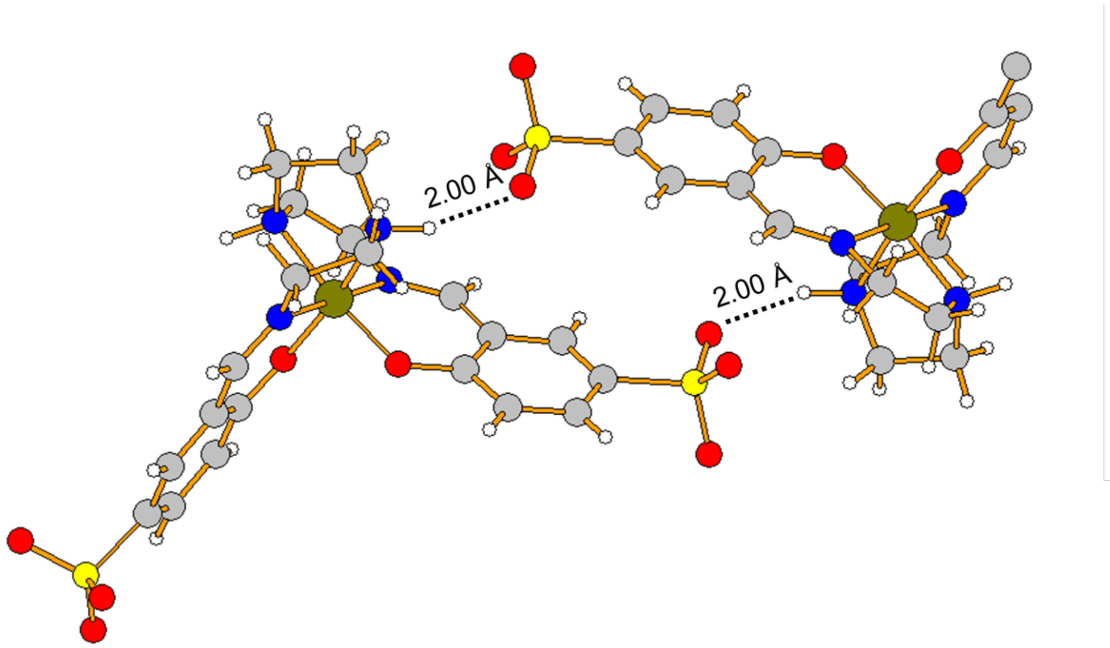
Chair: Jihyun Jang (Sogang University)

Design of Fe complexes with hydrogen-bonding-dependent spin equilibrium for Stable Aqueous Redox Flow Batteries

Donghwi Ko, Hye Ryung Byon[*]

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

Fe-based compounds in aqueous redox flow batteries typically exhibit high redox potentials and are mainly used as posolytes. To develop an all-Fe redox flow battery, it is necessary to develop negolyte materials with lower redox potentials. Phenolate moieties have been employed to reduce the redox potential of Fe complexes due to their π-donor and strong Lewis base properties. However, these ligands primarily form Fe complexes in the high-spin state with weaker binding affinity, leading to low electrochemical stability.In this study, we introduced a secondary amine group capable of forming strong σ bonding with the Fe metal center under aqueous conditions. Additionally, sulfonate groups on phenolate rings were utilized to facilitate intermolecular H-bonding with neighboring secondary amine groups, enhancing the σ bonding between amines and irons and promoting molecular clustering. We also investigated a Fe complex including hydroxyl groups on phenolate rings as a control group, which cannot form intermolecular H-bonding and molecular clustering, as confirmed by SAXS measurement. Evans method and Raman analysis confirmed higher effective magnetic moment values and weaker metal-ligand binding affinity for the hydroxylated Fe complex. Cyclic voltammetry and aqueous redox flow battery measurements demonstrated superior electrochemical stability for the sulfonated Fe complex compared to the hydroxylated one, which decomposed rapidly. Furthermore, the sulfonated Fe complex exhibited high solubility in water at 0.7 M and demonstrated stable cycling of the redox flow battery for 300 cycles in a neutral aqueous electrolyte at a concentration of 0.5 M.


2.00 Å
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Oral Presentation : **EDU.O-1**

New Trends in Chemistry Education

Room 404 THU 09:00

Chair: Hyunjung Kim (Kongju National University)

Teaching and Learning Strategies with Chat Artificial Intelligence for Socio scientific Issues' Problem-solving

HyunJu Park

Faculty of Chemistry Education, Chosun University, Korea

The purpose of this study was to investigate the educational use of artificial intelligence (AI). Through its ability to analyze and integrate vast amounts of data, generative AI can gather information about socio-scientific issues (SSI) from a variety of sources. Based on this, it can propose a comprehensive and detailed framework for teaching socio-scientific issues. Big data can also provide new perspectives and ideas beyond the traditional human-centered approach. Generative AI can also quickly respond to evolving scientific discoveries and social issues. These capabilities will keep the SSI framework up to date and provide timely educational resources. This study analyzed the educational value of generative AI by examining the differences between SSI frameworks developed by science educators and generative AI. The use of generative AI in the development of SSI frameworks could provide a different dimension of analysis than traditional approaches, contributing to the exploration of new ways to address SSIs in science education.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

New Trends in Chemistry Education

Room 404 THU 09:20

Chair: Hyunjung Kim (Kongju National University)

A study on the applicability of a project-based learning method in college sustainability education courses

Sukjin Kang

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

In this study, the applicability of a project-based learning method in college sustainability education courses for prospective teachers were investigated. Twenty-three senior students from a university of education participated in this study. A pre-test on environmental behavior and attitudes were administered followed by a five-week implementation of the sustainability education intervention during which students individually executed energy-saving projects. A post-test, utilizing the same questionnaire as the pre-test, was administered. Additionally, individual interviews were conducted with nine students actively engaged in the projects. The analysis of interview content, portfolios, and reports identified sub-concepts related to program effectiveness and its causes, which were then organized into subcategories. Relationships recurring among subcategories were extracted to formulate a tentative explanatory model. Results indicated that the sustainability education intervention exerted positive impacts on students' pro-environmental behavior, values, and attitudes. Educational implications are discussed.

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

New Trends in Chemistry Education

Room 404 THU 09:40

Chair: Hyunjung Kim (Kongju National University)

An Analysis of Pre-service Chemistry Teachers' Questions in Their Teaching Practices Considering the Context of Discourse

Sunghoon Kim, Minhwan Kim[1], Taehee Noh[1,*]

Center for Educational Research, Seoul National University, Korea

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

In this study, pre-service chemistry teachers' questions in their teaching practices were analyzed considering the context of discourse. Five pre-service teachers participated in the study. Their questions were analyzed by considering various data including class videos, interviews, and teaching-learning materials. Their questions were classified into relevant question, affective question, dead-end question, rhetorical question, and structuring question. Each question was also classified into appropriate question and convenient question by the aspect of proper responses of students. The analyses of the results indicate the differences in the frequencies of several types of questions depending on the content of the lessons. After using convenient questions, pre-service teachers proceeded to prepared classes as they rather than prompted students' responses. The affective questions were rarely used. The dead-end questions were found to be used for promoting interaction with students. The rhetorical questions were used for various purposes such as arousing students' attention or promoting their thinking. Practical implications were discussed based on the results.

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Oral Presentation : **EDU.O-4**
New Trends in Chemistry Education
Room 404 THU 10:20
Chair: Hyunjung Kim (Kongju National University)

Organic Chemistry in High School Chemistry Curriculum

Jinho Oh

Chemistry & Biology, Korea Science Academy of KAIST, Korea

Chemistry is the study of matter and its changes. Matter is categorized into organic and inorganic compounds. Organic compounds are widely used not only in chemistry but also in various fields such as life sciences, chemical engineering, material science, materials engineering, and medicine. In addition, we encounter organic compounds in our daily lives. Organic chemistry, which deals with organic compounds, is a required undergraduate course in chemistry and related disciplines. However Organic chemistry is considered a difficult subject for non-chemistry majors.Should organic chemistry be taught in high school chemistry courses? And if so, how should it be taught to high school students? In Korea, fundamental organic chemistry has been taught as an elective course for chemistry enrichment. We will look at how organic chemistry is taught in high school chemistry curricula in Korea and abroad. We will discuss whether organic chemistry should be taught to high school students and, if so, how it should be taught.

133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

New Trends in Chemistry Education

Room 404 THU 10:40

Chair: Hyunjung Kim (Kongju National University)

Educational Implications of International Science Fairs for High School Students

Eun-Young Choi[*], **Duangkhae Srikun**[1]

Chemistry & Biology, Korea Science Academy of KAIST, Korea

[1]*Department of Chemistry, Mahidol Wittayanusorn School, Thailand*

Science fairs aligned with green chemistry and a cleaner world offer students opportunities for research presentation and exchange, thereby fostering their motivation for research towards a better future. Additionally, they offer a platform to enhance students' ability to present their research to others and develop communication skills. Moreover, international science fairs not only facilitate the exchange of diverse research findings but also provide a platform for cultural exchange, fostering improvement in language proficiency, and opportunities to make friends. These days, I believe that motivation is more crucial than simply acquiring knowledge in the educational setting. Through participation in science fairs, both teachers and students can find the motivation to engage passionately in inquiry. By interacting with international students, they can develop friendships and actively engage in exchanges, fostering an enjoyable environment for learning English and acquiring communication skills. I think there is a strong determination to learn these skills in order to communicate effectively. In line with future trends in education, I consider global interactions, both online and offline, to be essential educational methods. I have participated in over 10 science fairs such as TISF, JSSF, ISSF, KVIS-ISF, etc., and have been involved in the KSASF hosted by KSA. This presentation aims to share insights gained from these experiences.


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

General Session

Room 403 THU 09:00

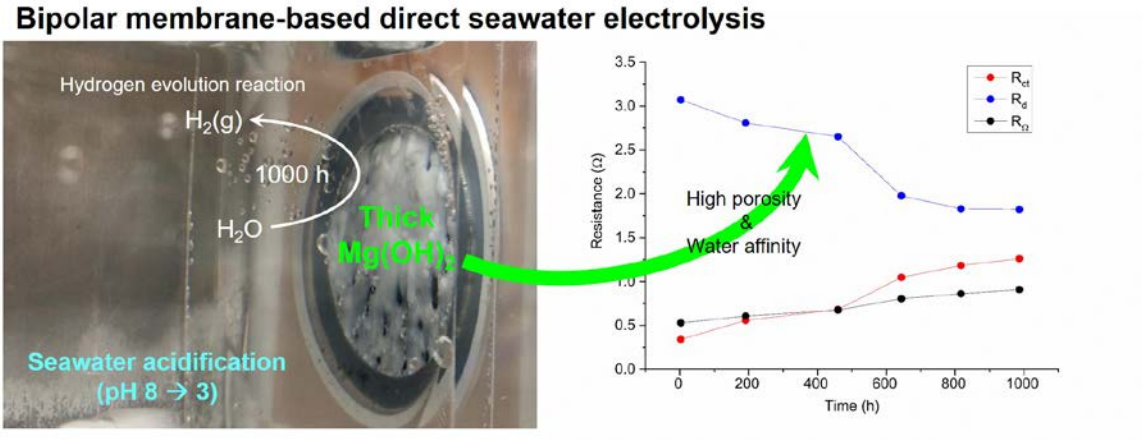
Chair: Eunju Kim (Seoul National University of Science and Technology)

Long-Term Stability of Seawater Acidification and Its Effect on the Formation of Mg(OH)2 Films with a Hierarchical Porous Structure in Bipolar Membrane-Based Direct Seawater Electrolysis

Jihyung Han

Korea Institute of Energy Research, Korea

This is the first report discussing the long-term stability (1000 h) of direct seawater electrolysis (DSWE) in relation to seawater acidification and inorganic precipitation. Unlike general DSWE, in which inorganic precipitates are formed at the cathode surface due to a local pH increase caused by the hydrogen evolution reaction (HER), bipolar membrane-based DSWE acidified natural seawater to pH 3, suppressing the formation of inorganic precipitates and inducing a positive shift in the equilibrium potential for the HER. Because the acidified seawater became alkaline after 300 h, periodic seawater replacement was suggested as a method of maintaining seawater acidification for 1000 h, during which a Mg(OH)2 film with a thickness of 1 mm or more was formed at the cathode surface. Using Brunauer–Emmett–Teller (BET) analysis, water vapor sorption, and electrochemical impedance analysis, it was confirmed that the Mg(OH)2 film has a hierarchical mesoporous structure and high affinity for water, which maintained mass transport. The unique properties of the Mg(OH)2 film under seawater acidification contributed to a lower rate of increase in the cathodic potential than that under seawater alkalization, where very thin inorganic deposits were formed.


Bipolar membrane-based direct seawater electrolysis
Hydrogen evolution reaction
$H_2(g)$
1000 h
H_2O
Thick $Mg(OH)_2$
Seawater acidification
(pH 8 → 3)
High porosity
&
Water affinity
R_{ct}
R_d
R_Ω
Resistance (Ω)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0
200
400
600
800
1000
Time (h)

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

General Session

Room 403 THU 09:30

Chair: Eunju Kim (Seoul National University of Science and Technology)

Optimized Raman system for nanoplastic detection

Dongha Shin

department of chemistry, Inha University, Korea

Raman spectroscopy is extensively utilized for measuring microplastics, yet it has considerable limitations for analyzing nanoplastics smaller than 1 micron. In this presentation, we'd like to introduce the development of a Raman spectroscopy system specialized in nanoplastic analysis, which is designed for versatile use across various applications.

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Oral Presentation : **ENVR.O-3**
General Session
Room 403 THU 10:00
Chair: Eunju Kim (Seoul National University of Science and Technology)

Understanding the Role of Structural Variance in Metal Oxide Photoelectrode Performance

Hye Won Jeong, **Hyunwoong Park**[1,*]

Advanced Institute of Water Industry, Kyungpook National University, Korea
[1]*School of Energy Engineering, Kyungpook National University, Korea*

The importance of developing efficient technologies for converting solar energy into chemical energy has drawn attention, particularly through solar water splitting using photocatalytic materials. It highlighted the complexity of factors affecting the performance of photoelectrodes in this process, including bandgap energy, carrier density, morphology, defects, and surface properties. Among them, nanostructuring in photoelectrodes offers the potential for improved efficiency due to their large specific surface area and accelerated charge transfer. Despite more than a decade of dedicated research into the impact of nanoscale morphology on the photoelectrochemical (PEC) performance of semiconductor materials, the literature still contains notable disparities and debates. This study aimed to provide clarifying comparisons of the effect of the shape and dimensions of particles in a photoelectrode. It explores various synthetic methods to control morphology, using titanium dioxide (TiO2) as a model material for testing. Surface analysis via XRD, Raman spectroscopy, XPS, etc. demonstrated that the chemical nature of the nanostructures is practically identical, and only morphology offers a difference in PEC performance. A comparison of morphology effects of PEC activities in sulfite and water oxidation gave insight into the dependence on particle morphology.This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (NRF-2022R1I1A1A01053034).

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

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

General Session

Room 403 THU 10:30

Chair: Eunju Kim (Seoul National University of Science and Technology)

Exploring Underlayer Modifications for Efficient Solar Chemical Conversion on Copper base Mixed Oxide Films

Seung Yo Choi, **Hyunwoong Park**[1,*]

Environmental Science Institute, Kyungpook National University, Korea

[1]*School of Energy Engineering, Kyungpook National University, Korea*

This study focuses on synthesizing copper-based delafossite films through electrodeposition on transparent conducting substrates (FTO) and investigates their photoelectrochemical (PEC) behavior and unassisted photocatalytic (PC) activities for solar chemical conversion in aqueous solutions. We observe that the surface property, crystalline structure, PEC, and PC performance for Solar chemical conversion are significantly influenced by the synthetic conditions. Optimized Cu-based delafossite catalysts exhibit suitable energetics for solar chemical conversion. However, we have identified a challenge with rapid electron-hole recombination in this copper-based delafossite material due to its narrow bandgap, posing a disadvantage in solar chemical conversion. To address this issue, we introduce a hole extraction underlayer deposited on FTO substrate for the catalyst. The primary roles of the underlayer are to establish a robust contact between the delafossite catalyst and substrates, facilitate hole transfer, and improve the deposition kinetics of the delafossite precursors. Additionally, the underlayer plays a secondary role in establishing firm contact between the substrate and catalyst. Through this underlayer, we were able to improve the Faradaic efficiency (F.E.), Solar-to-chemical conversion (STC) efficiency and selectivity of solar chemical conversion. Furthermore, we provide clear insights into the interests through Density Functional Theory (DFT) calculations. This research was supported by the National Research Foundation of Korea (RS-2023-00246948).

Poster Presentation : **POLY.P-1**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Polymerization of mesogenic monomers based on the thiol-ene system

Thu Loan Dang, Hyeonuk Yeo[1,*]

Department of Chemistry, Kyungpook National University, Korea

[1]*Department of Chemistry Education, Kyungpook National University, Korea*

Following the well-known concept of ‘click’ chemistry, the radical-mediated thiol-ene reaction exhibits as one suck ‘click’ reaction. In particular, this reaction provides all the desirable features like being highly efficient, simple to execute with no side products and proceeding rapidly to high yield. While the majority of the thiol-ene studies pursue photo-initiated pathways, thermal polymerizations under different curing conditions will be investigated in this research. Here we firstly report the synthesis and characterization of a series of liquid crystalline diallyl ethers as monomers based on different aliphatic spacers. These monomers were successfully synthesized from biphenol as a mesogenic ingredient, and then 1H-NMR spectroscopy, differential scanning calorimetry (DSC) and polarized optical microscopy (POM) measurements were performed to analyze functional groups, phase transition behaviors and mesophase texture, respectively. Afterwards two systems of the mesogenic dienes and either bi-functional or tetra-functional thiols were thermally polymerized in the presence of an organic peroxide serving as a pertinent free-radical initiator. As a result, two systems of thermoplastic and thermosetting polymers were auspiciously tailored and disclosed enhanced thermal properties.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancement of thermal conductivity and mechanical properties of liquid crystal epoxy resins through unique monomer design and systematic selection of curing agents

Thi En Trinh , Hyeonuk Yeo[1,*]

Department of Science Education, Kyungpook National University, Korea

[1]*Department of Chemistry Education, Kyungpook National University, Korea*

Liquid crystal epoxy resins (LCERs) emerge as dominant candidates for high heat-dissipating thermosets, tackling the heat accumulation challenge in modern electric devices. LCERs maintain the ordered polymer network structure after curing the monomer in the liquid crystal (LC) state with a suitable curing agent, ensuring retention of the LC structure in the final networks. The monomer and curing agent design, along with the curing temperature, crucially determine thermal conductivity. Herein, a unique monomer epoxy design based on Biphenyl mesogen, cured with special agents at an optimal temperature, maximizes microcrystal structure retention. Consequently, resulting thermosets boast superior thermal conductivity (up to 0.75 W/mK) and robust mechanical properties. Additionally, The study delves into multifactorial aspects influencing the cured network structure. These findings offer a pathway for fabricating high-performance materials for the electric industry.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Thermal and Optical Activities of Mesogenic Isosorbide-rooted Polyepoxides

Minh Hoang Le, Kyosun Ku[1], Hyeonuk Yeo[2,*]

Department of Chemistry, Kyungpook National University, Korea

[1]*Advanced Institute of Water Industry, Kyungpook National University, Korea*

[2]*Department of Chemistry Education, Kyungpook National University, Korea*

Derived from the humanistic demand of replicating and cloning nature, asymmetric chemistry has become one of the modern attentive research fields. The studies of chiral polymers therein are promising with the aspiration of representing the characteristics of natural macromolecules. We modeled a chiral polymer using an isosorbide core, following a straightforward crafting strategy by both identical and distinct substituents. Mesogenic fractions were employed to gain advantages of its well-known highly ordered structure to enhance the crystallinity and alignment of the polymer. Aromatic amines and imidazolium initiators were operated for an advantageous curing process and the insertion of crosslinks to the materials. Thermal properties of the obtained copolymers were formerly measured and analyzed accordingly. Supplementary research offered the treatment of uniformly mesogenic polymers to enhance their liquid crystallinity.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancing wound healing by tuning the mechanical properties of lignin/zwitterionic polymer-based multifunctional hydrogels

Yiluo Hu, Jaewon Choi, Younsoo Kim*

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

Tissue adhesives have attracted widespread interest as alternatives to supplements of sutures, but significant challenges remain, including weak tissue adhesion, inadequate biocompatibility, and uncontrolled biodegradation. In this study, we developed an adhesive lignogel with excellent cohesion and adhesion abilities through cation-pi interaction between biopolymer lignin and zwitterionic polymer. Lignogel was prepared by irradiating microwaves to an aqueous solution of lignin and zwitterionic polymers. The obtained gel showed various viscoelastic properties and electrical conductivity depending on the composition concentration. When the concentration of lignin and polymer was low, adhesion was excellent, but toughness was low. As concentration increases, toughness increases, but surface adhesion decreases. Therefore, different concentrations of lignogel were mixed to ensure strong adhesion to biological tissues and thus accelerate wound healing. These lignogels offer tremendous potential in surgical applications such as non-suture wound closure and hemostatic closure. In this presentation, we introduce the synthesis strategy of lignogel, its characteristics, and biological applications.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis and properties of cyclic olefin polymers using various functional groups based on oxanorbornene derivative

Huigyung Kim, Kyosun Ku[1], Hyeonuk Yeo[2,*]

Depart of chemistry, Kyungpook National University, Korea

[1]Advanced Institute of Water Industry, Kyungpook National University, Korea

[2]Department of Chemistry Education, Kyungpook National University, Korea

Cyclic olefin polymers (COPs) and cyclic olefin copolymers (COCs) are widely used thermoplastic engineering materials. Unique optical, electrical, thermal, and mechanical properties of COP make them utilized in a variety of areas including optical parts for digital cameras and laser beam printers, optical recordings, medical products, and electrical insulation applications. In this study, the COPs are synthesized by ring-opening metathesis polymerization (ROMP) of the poly cyclic olefins followed by hydrogenation of double bonds. The chemical structures are confirmed by HNMR, CNMR and the molecular weights of the polymer are investigated by GPC analysis. In addition, thermal properties are investigated using DSC measurements. Further, in the presentation, optical properties of the COPs through Uv-vis will be investigated in details.

Poster Presentation : **POLY.P-6**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Design of reprocessable high-functional bismaleimide vitrimer

Woohyeon Kwon, Kyosun Ku[1], Hyeonuk Yeo[2,*]

Department of Chemistry, Kyungpook National University, Korea
[1]*Advanced Institute of Water Industry, Kyungpook National University, Korea*
[2]*Department of Chemistry Education, Kyungpook National University, Korea*

Bismaleimide (BMI) resin is a family of high-performance thermosetting material mainly used in extreme environments such as aerospace field due to its excellent physical, chemical, and thermal stability. However, despite these excellent advantages, it has some disadvantage that re-processing or recycling is merely not possible. Therefore, it becomes permanent waste after use and cause severely environmental issues. To solve this problem, a new BMI vitrimer system with exchangeable ester bonds was designed and synthesized. The chemical structures of the synthesized monomer were verified using 1H NMR, 13C NMR, and FTIR spectroscopy. In addition, the thermal properties of the cured vitrimer based on the synthesized monomer were investigated through DMA, TGA, and DSC. Further, reprocessing process of the cured vitrimer was carried out. The properties of reprocessed specimens obtained after the heat pression remolding were investigated and comparative analysis was performed to verify the reprocessibility of the designed BMI vitrimer system.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

A Study on the Improvement of Thermal Conductivity of PEG-based Liquid Crystal Thermoset

Kyosun Ku, Hyeonuk Yeo[1,*]

Advanced Institute of Water Industry, Kyungpook National University, Korea

[1] *Department of Chemistry Education, Kyungpook National University, Korea*

With the development of nanoscience and nanotechnology, the thermal density in the circuit is continuously increasing, and the demand for thermal management materials is increasing. In particular, polymer materials have various advantages such as low cost, high processability, and insulation, but there is a limit to the application of electronic materials due to their low thermal conductivity. In this study, we conducted study to improve thermal conductivity by using the molecular assembly properties of liquid crystal polymer (LCP). The microstructure of LCP depending on the alkyl spacer are investigated. The microscopic orientation properties are inspected by XRD and POM. Thermal properties investigated by DSC, TGA, and DMA. The thermal conductivity of the synthesized LCP recorded a higher level of thermal conductivity (~ 0.5 W/m·K) than the conventional polymer. The temperature change was observed by a thermal imaging camera to confirm the thermal conductivity of LCP.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Oxidation-induced Biocompatible Poly(PG/Amine) Coating: Formulation for Black Hair-Dyeing

Nayun Kim, Woo Kyung Cho[1,*]

Chungnam National University, Korea

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

Hair dye shampoos have been developed by harnessing the natural oxidative principle inspired by the browning phenomenon observed in fruits and plants, utilizing plant-derived polyphenolic compounds. In this study, we explored the use of readily available polyphenolic molecules for the formation of oxidation-based coatings for hair dyeing. Pyrogallol (PG), chosen for its high oxidative power and biocompatibility, is identified as a promising compound for this purpose. The optimization of oxidation-induced PG coating for hair dyeing is achieved through the use of amine cross-linkers. The optimal amine molecule and molar ratio between the amine and PG was determined to achieve the highest coating efficiency and dark black-brown color. The optimal conditions were then employed for hair dyeing and the subsequent assessment of hair dye stability. We believe that this study provides valuable insights into the chemistry of polyphenols and their practical applicability in cosmetics and pharmaceuticals.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis and Application of Glycol Chitosan-Based Antimicrobial Agents: An Approach to Treat Healthcare-Associated Bacterial Infections

Sunhee Kim, Kang Moo Huh[1,*], Woo Kyung Cho[*]

Department of Chemistry, Chungnam National University, Korea

[1]*Department of Polymer Science and Engineering, Chungnam National University, Korea*

Bacterial infections present a significant risk due to their rapid multiplication and the release of toxins, leading to tissue damage and potential systemic disease. Severe cases can escalate into life-threatening conditions, including sepsis, as infections spread throughout the body. The emergence of antibiotic-resistant bacteria further complicates treatment, heightening the risk of prolonged illness and increased mortality rates. As innovative antimicrobial agents, we synthesized glycol chitosan-based quaternary ammonium materials via aza-Michael reactions between glycol chitosan and various quaternary ammonium salts, each with distinct hydrocarbon chain lengths. Four derivatives were synthesized and characterized using $_1$H NMR spectroscopy. Antimicrobial effects and cytotoxicity of the derivatives were examined through the colony forming unit method and WST-8 assay, demonstrating that the materials with specific hydrocarbon chain length exhibit non-cytotoxicity and excellent antimicrobial properties. We believe that the quaternary ammonium derivative has high potential in treating healthcare-associated bacterial infections.

Poster Presentation : **POLY.P-10**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Tyrosinase-Mediated, One-Pot Zwitterion-Codeposited Eumelanin Coatings for Antibacterial Applications

Jong Hyeon Byeon, Woo Kyung Cho*

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Inspired by natural melanogenesis, we have devised a one-pot zwitterionic coating approach mediated by tyrosinase for antibacterial applications. In this study, amine-terminated sulfobetaine (SBAm) and carboxybetaine (CBAm) were successfully synthesized and grafted onto surfaces through Michael addition and Schiff base reactions with enzymatically oxidized tyrosine, utilizing its catecholamine group as a coating precursor. The surface coatings were characterized by spectroscopic ellipsometry, water contact angle goniometry, and X-ray photoelectron spectroscopy. The results demonstrated that the tyrosinase-mediated coatings can be formed in a substrate-independent manner. The incorporation of zwitterionic moieties within the SBAm/CBAm-eumelanin films effectively inhibited bacteria adhesion against E. coli. We believe that this simple and versatile coating method can be used on demand and holds significant promise for biomedical applications where biofouling prevention is crucial.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

An Easy-handling Approach to Antimicrobial Coatings for Medical Devices : One-pot Complexation of O-Carboxymethyl Chitosan and Zirconium Chloride

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This study presents a surface modification method utilizing O-carboxymethyl chitosan (O-CMC) and zirconium chloride ($ZrCl_4$) to develop antimicrobial coatings for medical devices. The formation of hydration layer, facilitated by hydrophilic nature of CMC/Zr(Ⅳ) complex coatings, effectively inhibits bacterial adhesion and biofilm formation on surfaces. The straightforward, one-pot coating process offers a practical advantage by eliminating the need for multiple steps. Various characterization techniques including ellipsometry, contact angle goniometry, X-ray photoelectron spectroscopy, field-emission scanning electron microscopy, and atomic force microscopy were employed to evaluate the coatings on diverse substrates. Antimicrobial experiments, antiplatelet tests, and enzyme-linked immunosorbent assay analyses confirm the efficacy of the antifouling coating, particularly on titanium substrates commonly used in implants. This surface modification approach holds promise in addressing the significant challenges associated with bacterial infections related to medical devices, potentially enhancing overall patient safety.

Poster Presentation : **POLY.P-12**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis of Waterborne Polyurethane for Reducing VOCs and Fabricating Fluorescent Pigment Compositions

Joon Kim, DaYe Kim, Seung Goo Lee[*]

Department of Chemistry, University of Ulsan, Korea

Polyurethane (PU) is one of the polymers widely used in everyday life and industry because it is easy to control its physical properties during the fabrication process. However, organic solvent-based PU demonstrates the disadvantage regarding the release of volatile organic compounds (VOCs) after the application, raising environmental and health concerns. In this study, an eco-friendly and waterborne polyurethane (WPU) is prepared using water as a solvent to mitigate the production of the existing organic solvent-based PU. The PU is generally not soluble in water, but this study proposes a method of introducing a hydrophilic compound into the PU structure and dispersing it in water. The WPU is synthesized using hydrophilic 2,2-bis (hydroxymethyl) butyric acid, isophorone diisocyanate, poly(tetramethylene ether) glycol 2000, a neutralizing agent, and a chain extender. The urethane bond is characterized using fourier transform infrared spectroscopy, the particle size is confirmed with dynamic light scattering, and the physical properties are systematically analyzed with a viscometer, a tensile strength meter, and differential scanning calorimetry. Finally, the synthesized WPU is dyed with coumarin and rhodamine-based fluorescent dyes to produce fluorescent pigments. We expect this technology to contribute significantly to the paint industry by introducing non-toxic and environmentally friendly WPU paints.

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Poster Presentation : **POLY.P-13**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Cr-free anti-corrosion eco-friendly composite inorganic coating agent

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The zinc contained in galvanized steel sheets is highly active and easily oxidized, so chromium compounds are used to increase the corrosion prevention effect. However, chromium compounds have the disadvantage of being harmful to the human body and the environment, so research into alternatives to chromium compounds is essential. In this study, we propose a chrome-free anti-corrosion eco-friendly coating solution using silica nanoparticles and sodium metasilicate, which have excellent anti-corrosion performance. A mixed solution of silica nanoparticles and sodium metasilicate was coated on a hot-dip galvanized steel sheet using a spray coating method. Solution synthesis and curing time were optimized through FT-IR analysis and pencil hardness testing. The thickness of the coating was adjusted according to the amount of sprayed liquid, and the thickness of the coating layer was checked and optimized using F-40. The corrosion prevention performance of the coated steel sheet was confirmed through the corrosion resistance (Rcorr) value obtained through the linear Tafel plot test of the potentiostat. Through this study, it is expected that the corrosion prevention performance of hot-dip galvanized steel sheets can be improved in a simple, human-friendly, and eco-friendly way.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Keratin-Based Acid-Resistant Protein Coating Technology and Its Mechanical and Chemical Properties

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Keratin is one of the most abundant materials readily available from natural resorces, including wool, hair, and hooves, which are byproducts of various organisms. In addition, keratin is both biodegradable and biocompatible, and boasts excellent acid-resistance and broad physical/chemical stability, particularly when compared to other biopolymeric materials. These distintive properties of naturally derived keratin can be leveraged to create films for direct application in acid-resistance coating. Film prepared via solvent casting, which holds the advantage of a very simple process. However, conventional keratin-only films are too vulnerable to water, necessiating additional cross-linking to overcome this issue. Yet, even after cross-linking, films are too brittle to be universally utilized. In this study, we aimed to mitigate this challenge by enhancing the alpha-helical conformation associated with the flexibility of regenerated keratin using citric acid. Furthermore, in the process of extracting keratin from human hair, we induced internal disulfide bond reconstruction within the keratin molecules using 1,4-dithiothreitol. This eliminated the need for post-cross-linking processes, whcih are the main cause of brittleness in the keratin films. This study therefore aims to utilize the unique advantages of keratin, such as the biocompatibility of the protein itself, to efficiently apply it as an acid-resistant coating material for food or biomaterials.Keywords: Keratin, Flexibility, Disulfide bond reconstruction, Acid-resistance

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Fabrication of Implantable Electrochemical Sensor using Biocompatible Conformal Coating Technique

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Implantable biosensors, designed to detect organ function or the body's state through minute changes in current or signals from the cells or tissues they come into contact with, have been extensively studied. Among these, electrochemical (ECS) signals are known for their high sensitivity and broad applicability to a variety of molecules, but their adoption has been limited due to the exposure of the intrinsic surface of the electrode, essential for reading electrical signals, to the living body. To address the physical and mechanical differences between electrodes and biological tissue, we aimed to introduce a technique to conformally coat the electrode surface with a biocompatible hydrogel. We used a self-healing hydrogel made of alginate oxide and gelatin amine cross-linked to the PDMS surface of a conductive electrode. The GelMA hybrid hydrogel with multi-walled carbon nanotubes (MWCNTs) as the conductive material was applied to the conductive electrode. This sensing component exhibits tissue-like mechanical strength and has a complex exchange interface for ions and electrons, enabling mechanical and electrical coupling with biological tissue. This technique will enable the development of sensors capable of reading electrochemical signals in vivo.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Sequence-defined polyester equipped with complementary H-bonding base-pair

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Sequence-defined synthetic polymer is a promising molecular media for permanently storing digital information. However, when the synthesized polymer with a defined sequence is exhausted, it must be synthesized again from monomers, which makes the process inefficient. Here, we demonstrate an efficient synthetic method by imitating biopolymers such as nucleic acids which synthesize polymers by chain replication through complementary bonds. We synthesized sequence-defined polyester containing adenine and thymine nucleobase by cross convergent method. Thymine and adenine were attached as side chains of the polyester backbone. A monomer with a soluble chain was inserted between the nucleobase monomers to increase solubility.

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Poster Presentation : **POLY.P-17**
Polymer Chemistry
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Polymer composites for interlayer sound insulation materials (ISIMs) with elasticity and insulation

Gibok Lee

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Poster Presentation : **POLY.P-18**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Deodorizing Methods for Recycled Polyolefin Plastic Wastes

Hyunhoon Kim

R&D Center, HDC Hyundai Engineering Plastics Co., Korea

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Selective Hydrogenation of Alkynes with Palladium Nanocatalysts in Poly(ethylene glycol)-Coated 3D-Continuous Nanoporous Membranes

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We developed palladium nanoparticles (Pd NPs)-loaded membrane with a three-dimensional (3D) continuous nanoporous structure. This structure was achieved by blending the cross-linked polyurea network (UN) sol with poly(ethylene glycol) (PEG), followed by solvent evaporation. Removal of the polymer component from the PEG/UN blends resulted in a 3D-continuous nanoporous membrane, where the skeleton and porous channel coexisted together continuously on the nanoscale, with the pore surface coated with PEG brushes bound to the UN domain. Within these 3D nanoporous channels, reduction of the Pd precursor along the PEG-coated pore surface produced ultrafine Pd NPs (1~2 nm in diameter) with their number density adjustable by varying metal precursor concentrations. The resulting Pd-loaded nanoporous membrane catalysts were tested in liquid-phase selective hydrogenation of alkyne. We observed their high catalytic activity and selectivity for desired alkene product, elucidating the high selectivity through the preferential adsorption of alkyne substrate over alkene.

Poster Presentation : **POLY.P-20**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Photo-Crosslinkable Single-Component Copolymers for Functional Coatings

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We demonstrate the design and synthesis of poly(ethylene oxide)-based random terpolymers, which possess a repeating unit with photolabile o-nitrobenzyl pendent group to release primary amine upon exposure to UV light, and amine-reactive functional groups of glycidyl or cyclic dithiocarbonate group capable of single-component functional organic coatings. Coatings prepared from terpolymers crosslinked by UV light were applicable to a variety of substrates from organic to inorganic. The resulting coatings were chemically versatile in immobilizing complex molecules on surfaces by (i) functionalized after crosslinking and mixing (ii) a specific protein that could form dual networks, namely fish skin gelatin, to form complex coatings. The resulting copolymerized coatings were thoroughly characterized to highlight their applicability to surface coatings and photolithographic applications by using a variety of functional molecules to obtain patterns with integrated specific functions, control surface wettability, or regulation of adhesion of biological objects.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis of Polymeric [2]-Catenanes Composed of Interlocked Discrete Cyclic Polymers

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Cyclic polymers have been extensively studied because of their unique physicochemical properties originated from their endless ring conformation. Discrete cyclic polymers can be synthesized via the combination of iterative exponential growth, end-group functionalization and intramolecular cyclization. In addition, polymer catenanes, composed of interlocked cyclic polymers, were prepared by the template threading approach. Using the linear convergent method, functional monomers were precisely placed into polymer chains. In this research terpyridyl functional group were placed into polymer chains to make metal-ligand interaction between two polymers. Because metal-ligand interaction connects two polymers, catenane synthesis can be performed efficiently.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Self-Healable, Stretchable, and Adhesive Ionogels Formed by CopolymerAssociation

Hyeon Ji Lee, Kim Seungjun, Myungwoong Kim[1,*]

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

We report the fabrication of self-healable, stretchable, and adhesive ionogels composed of two types of copolymers having hydrogen bond acceptors and donors, and an ionic liquid. A series of ABA triblock copolymers composed of an IL-phobic A block and an IL-philic B block is designed and synthesized. The copolymers form micelles through IL-phobic interaction of the A block, and the micelles are associated through the hydrogen bonding of the corona B blocks. These interactions can be controlled by different type of the copolymer with functional groups which can make additional hydrogen bonding. The resulting ionogels exhibit decent elasticity and adhesion capability to the surfaces of various materials. Moreover, the ionogels were capable of recovery from the physical damages at at room temperature. With their ion conductive properties, the resulting ionogels are further subjected to the electronic applications such as an electrolyte-gated organic thin film transistor and a motion sensor.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Cationic Polymerization of Epoxy-Containing Monomers Using Structurally Varied Thermal Initiators in a Flow Mode.

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Latent initiators, which are activated by specific external stimuli such as heat and illumination of light with a specific wavelength, allow their initiation to generate activated species for polymerization under desired conditions. However, readily activated latent initiators used in the polymerization can often lead to extremely exothermic and uncontrollable reactions. To address these issues, the polymerization in a flow mode is often employed. In the flow chemistry, effective heat transfer in the flow can prevent the uncontrolled reaction. Herein, we present cationic polymerization of an epoxy-containing monomer, which was known to be highly exothermic in a conventional batch mode, can be controlled in a flow mode. The activity of the initiator is studied by probing polymerization kinetics with modifying the chemical structure of ionic sulfonium compounds to understand the structure-activity relationship of various initiator-epoxy monomers in a flow mode. Furthermore, we attempted to expand the feasibility of thermal cationic polymerizations with other monomers than epoxy-containing monomers.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Shotgun sequencing of 512-mer copolyester allows random access to stored information

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Digital information encoded in polymers has been exclusively decoded by mass spectrometry. However, the size limit of analytes in mass spectrometry restricts the storage capacity per chain. In addition, sequential decoding hinders random access to the bits of interest without full-chain sequencing. Here we report the shotgun sequencing of a 512-mer sequence-defined polymer whose molecular weight (57.3 kDa) far exceeds the analytical limit of mass spectrometry. A 4-bit fragmentation code was implemented at random positions during the synthetic encoding of 512-bit information without affecting storage capacity per chain. Upon the activation of the fragmentation code, the polymer chain splits into 18 oligomeric fragments, which could be individually decoded by tandem-mass sequencing. These sequences were computationally reconstructed into a full sequence using an error-detection method. The proposed sequencing method eliminates the storage limit of a single polymer chain and allows random access to the bits of interest without full-chain sequencing.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis and Crystallization-Driven Self-Assembly of Block Copolymers Composed of Stereoregular Poly(mandelic acid) and Poly(ethylene glycol)

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Poly(mandelic acid) (PMA) is structurally similar to polystyrene (PS) having a high glass transition temperature (Tg), and thus is stable even at a relatively high temperature. In addition, PMA having a stereoregularity has crystallinity. In the case of crystalline polymer, a controlled low-dimensional structure that may not be seen in the self-assembly behavior of an amorphous polymer can be observed. Herein, we report the synthesis of block copolymers composed of discrete stereoregular poly(mandelic acid) and poly(ethylene glycol). Furthermore, We can compare the CDSA behaviors according to the controlled stereoregularity and the chain length of poly(mandelic acid). It is expected that this work allow us to understand the crystallization of PMAs and enable more precise polymer nanostructure design.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Self-Assembly of Discrete Amphiphilic Cyclic Block Copolymers based on Poly(α-hydroxyglutaric acid)

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Self-assembly of amphiphilic block copolymers in selective solvents is a broad research field due to the significant potential applications of the resulting nanostructures such as drug delivery. Previous studies have shown the effect of polymer topology on self-assembly behavior among various factors. In particular, the cyclization of amphiphilic block copolymers can result in unique self-assembly behavior. Unlike linear block copolymers, cyclic block copolymers self-assemble compact and entropically disfavored nanostructure owing to its loop-like structure. In addition, self-assembly of cyclic block copolymers may impart improved properties such as greater thermal stability and robustness to the resulting nanostructures. Herein, we self-assembled amphiphilic cyclic block copolymers composed of discrete number of orthogonally protected monomers based on α-hydroxyglutaric acid with butyl and benzyl side-chain substituents. The monomers were derived from L-glutamic acid by selectively protecting butyl and benzyl groups to the carboxyl group at the γ-position, and then converting the amine to hydroxyl group via diazotization-hydrolysis reaction. For iterative exponential growth, the residual hydroxyl and carboxyl groups were protected by tert-butyldimethylsilyl and allyl groups, respectively. Amphiphilic block copolymer was cyclized via copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction, and hydrogenolysis of the benzyl group was finally performed to expose carboxylic acid for hydrophilicity.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Grafting-With Approach: Iterative Synthesis of Sequence-Defined Bottlebrush Polymers via Passerini 3-Component Reaction

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Bottlebrush polymers (BBPs) have unique physical properties due to the densely grafted polymeric side chains installed to the polymeric backbone. The synthesis of perfectly discrete BBPs allow precise estimation of absolute molecular weight characterized using analytical methods including light scattering. By employing iterative exponential (IEG) and grafting-to approach involving post-functionalization of side chains to reactive pendant groups tethered to the backbone, structurally defined BBPs with discrete side chains can be synthesized. However it remains a challenge because of the inherent steric hindrance despite the utilization of robust click coupling reactions, resulting in incomplete grafting of polymeric side chains. In addition, synthesis of sequence-defined discrete BBPs is challenging due to the limited orthogonal click reactions reported thus far.In this project, a novel strategy involving simultaneous grafting of side chains onto the growing polymeric backbone via the combination of iterative exponential growth (IEG) and Passerini- three component) (P-3CR) reactions was studied. Amongst the three components, carboxylic acid (-COOH) and aldehyde (-CHO) groups were orthogonally protected with 1,3-dithiane and allyl ester groups, respectively. The orthogonally protected monomers coupled with cyclohexyl isocyanide via P-3CR reaction, followed by subsequent orthogonal deprotection and P-3CR reactions, to afford homopolymer containing up to 63 repeating units. The facile side chain functionalization demonstrated the potentiality of mitigating steric hindrance associated with the installation of polymeric side chains, in addition, serves as a potential platform for tailoring defined complex molecular architectures including concave and ellipsoid geometries.

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

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Distinct Thermoresponsive Properties of Nanostructured Poly(*N*-isopropylacrylamide)

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Herein, we present the end-group effect on the thermoresponsivity of poly(*N*-isopropylacrylamide) (PNIPAM) nanostructures. In this study, nanostructured PNIPAM having three different end-groups were prepared in the form of block copolymer (BCP) micelles or surface-modified gold nanoparticles (AuNPs). Due to the closely arranged end-groups exposed at the periphery of nanoparticles, the electrostatic and hydrophobic interaction between the end-groups significantly affect the thermoresponsive properties of PNIPAM nanoparticles. For instance, negatively charged end-groups increase the electrostatic repulsion between PNIPAM nanoparticles, preventing aggregation even above the lowest critical solution temperature (LCST). On the other hand, hydrophobic end-groups enhance the hysteresis effect by promoting stronger hydrophobic interaction among PNIPAM nanoparticles. Furthermore, PNIPAM-stabilized AuNPs, having high hysteresis and heat-induced extinction/color difference, were applied to create a heat-derived color display. These findings highlight the significance of the end-group in determining the temperature-dependent behavior of nanostructured PNIPAM, regardless of the core material used.

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Poster Presentation : **POLY.P-29**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Cellulose Composite Microbeads with Covalent Organic Nanosheets

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Microplastics, including microbeads, which are widely used for industrial purposes as well as daily necessities such as detergents, toothpaste, and cosmetics, are becoming a serious environmental issue due to their non-degradable nature. If they accumulate in aquatic organisms, microplastics can eventually enter the human food supply chain and pose a risk to humans. Herein, we demonstrate a method to fabricate abundant, sustainable, and biodegradable microbeads though an electrospray process of cellulose acetate and subsequent chemical process as a sustainable alternative to microplastic particles widely used in various consumer products in our daily lives. In addition, the poor mechanical properties that degrade the potential of cellulose can be dramatically enhanced by incorporating triazine-based covalent organic nanosheets (CONs). The compressive strength at break of the composite microbeads was measured to be 238 ± 18 MPa, which is higher than that of cellulose microbeads without CON (142 ± 22 MPa) and polypropylene microbeads (199 ± 6 MPa). Our study proposes a simple yet effective approach to fabricate cellulose microbeads with improved mechanical properties, providing insight into how to replace petroleum-based microbeads with eco-friendly material systems.

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Poster Presentation : **POLY.P-30**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Vinyl-Addition Polymerization of 5-Vinyl-2-norbornene with Palladium(II) Catalyst

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VA-COPs has many advantages in polymer properties due to its bicyclic backbone. Though, their limited mechanical properties and lack of functionality constrain their various applications. Polymerization of polar monomers presents a potential solutions, but, it is accompanied by a reduction in catalyst activity. Here in, COP platform using VNB monomer is proposed for achieving variable polymer properties, which can be accomplished by modulating of molecular weight, functionality, composition, topology. VNB, a cost-effective cyclic olefin monomer, allows for further modification to impart various functionalites. However, branched PVNB is formed due to its divinyl nature and less chemo-selective polymerization. In this study, Palladium(II)-based catalyst system is designed, and a series of kinetic study is investigated for the synthesis of well-defined PVNB.

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Poster Presentation : **POLY.P-31**

Polymer Chemistry

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Fast and Large Motion of Self-Oscillating Gels based on High Diffusivity Induced by Phase-separated Structures

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Unlike conventional stimuli-responsive gels, self-oscillating gels can spontaneously repeat swelling/de-swelling without on-off switching of external stimuli by inducing the Belousov- Zhabotinsky (BZ) reaction. However, the degree of mechanical oscillation of the gel was usually small and slow. In addition, for the overall mechanical oscillation of the gel, the size of the gel must be smaller than a chemical wave of several hundred micrometers. Furthermore, the BZ reaction required strong acidic conditions, and the duration of this reaction was short. These problems could be overcome by using specific hydrated protic ionic liquids (PILs) as an alternative medium for the BZ reaction. However, no oscillation was observed in conventional self-oscillating gels because of the low diffusivity of the BZ substrates into the gels in the highly viscous solution, such as hydrated PILs.Herein, we designed novel self-oscillating gels showing fast and large deformation by tuning the internal structure of the gels. Using the collapsed form of poly(N-isopropylacrylamide) in a salt solution, it is possible to synthesize the phase-separated structures showing fast and large shrinkage of the gels. Interestingly, our phase-separated gels can oscillate even in a highly viscous solution owing to its high diffusivity. Also, our gel exhibited a fast propagation rate and long wavelength of the chemical wave. Thus, even in centimeter-scale bulk gels, overall swelling/de-swelling oscillations could be exhibited, an unprecedented oscillation that significantly improved the dimension of oscillations. Using this oscillation, our gel functions as a water pump, absorbing and

expelling water according to the flow of the oxidation wavelength. As a result, it shows the behavior of the swimming actuator moving forward in a specific direction.

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Poster Presentation : **POLY.P-32**
Polymer Chemistry
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Synthesis of Poly(3-Hexythiophene) & Poly(Dimethylsiloxane) Based Block Copolymers and Its Thermoelectric Properties

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Poly(3-hexylthiophene) (P3HT) is a polymer material used in various fields such as light-emitting diodes, organic field effect transistors, and organic optoelectronic devices because it has good physical properties such as high electroconductivity, optical properties, and also it is easy to polymerize and the structure of the monomer is easily changed. However, despite the hexyl group in 3-position, P3HT with high molecular weight has a rigid structure with pi-pi stacking. The low solubility from this structural characteristic, the plasticization after polymerization remaining limitation of related researches. In this study, we reports an attempt to block copolymerize P3HT with Poly(dimethylsiloxane) (PDMS), which was known as very flexible polymer. Di-, and Triblock copolymer was produced via Copper(I)-catalyzed azide-alkyne cycloaddition after polymerization of each block. And we also reported novel approach to synthesize this block copolyer using PDMS-Nickel macroinitiator. The electrical properties of the block copolymers are also reported.

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Poster Presentation : **POLY.P-33**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Revealing the charge transport mechanism in trap-assisted hydrogen-generating semiconducting polymers via two-step polymerization

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Polymer-based semiconducting polymers are receiving mass attention because of their large tunability in the hydrogen evolution field. Recently, polymer-based catalysts that convert solar energy into chemical energy have being widely studied. However, many researchers are mainly focused on applying organic semiconducting polymers, which have already been reported in various fields since the working mechanism of water splitting semiconducting polymers is not clear. In this report, 2,1,3-Benzothiadiazole (BT) based polymer catalysts were synthesized using Stile coupling, followed by Suzuki-Miyaura coupling reaction. The syntheses were carried out by simply controlling the order of water addition in the reaction system. The existence of BDT in the polymers was confirmed using 1H-NMR and UV-vis spectroscopy. Also, using time-correlated single-photon counting (TCSPC) spectroscopy, the generated charges were tracked. TCSPC data showed that the generated charges were transported from the BT-fluorene domain to the BT-BDT domain, and these charges were finally quenched by water in the reaction media to generate hydrogen gas. For the first time, a trapped-assisted hydrogen evolution mechanism was proposed and we believe these results could promote the development of newly designed photoactive semiconducting polymer catalysts.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Dual Trapping of a Metastable Planarized Triarylborane π-System for Seeded Polymerization

Heekyoung Choi, Soichiro Ogi[1,*], Naoki Ando[2], Shigehiro Yamaguchi[1,*]

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We report the kinetically controlled supramolecular polymerization of boron-containing π-conjugated molecules, which was enabled by a seeding method based on dual trapping of a metastable state by synergistic intramolecular hydrogen bonding and Lewis acid-based complexation. Planarized triarylborane-based molecule, which bears a diamide chain with chiral alkyl groups, was synthesized. Upon cooling, the solution of monomer afforded a supramolecular polymerization in a cooperative manner to form helical supramolecular nanostructures with intense J-type aggregate emission. In the presence of pyridine, the triarylborane moiety formed a Lewis acid-base complex, which enhances the stabilization of the metastable monomeric state. An assembly incompetent structure with a folded diamide chain conformation and a pyridine moiety axially coordinated to the boron atom is responsible for slowing the spontaneous aggregation. The seeding method was successfully applied to the solution to produce homogeneous nanofibers even at a high (millimolar-level) concentration. This unprecedented kinetic control via dual trapping provides an effective method to achieve seed-initiated polymerization under concentrated conditions.

Poster Presentation : **POLY.P-35**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Characterization of crystalline poly(ethylene)glycol hydrogels crosslinked with sub-units

Jungju Ryu[*], **Daewon Sohn**[1,*]

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

Structures and properties of crystalline poly(ethylene)glycol (PEG) hydrogels were investigated to understand the crosslinking effects on PEG macromer gels. In this study, PEG gels were prepared with linear- and star-macromers. The end groups were crosslinked by the radical reaction of diacrylate and catechol-based crosslinking. Crystalline behaviors of various star-PEG and linear-PEG gels were observed using differential scanning calorimetry (DSC). The PEG gels established a crystalline structure at around 20 C, which is lower than that of the original catechol-modified polymer. Rheological properties of the gels were observed upon temperature ranges. SAXS measurements explore the crystalline structures and demonstrate the structure-property relationship. The results reveal that the structure and property are controlled by subunit assembly.

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Poster Presentation : **POLY.P-36**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Functional Group-Dependent Proton Conductivity of Phosphoric Acid-Doped Ion-Pair Coordinated Polymer Electrolytes: A Molecular Dynamics Study

Hyeonju Lee, **Hyungjun Kim**[*]

Korea Advanced Institute of Science and Technology, Korea

Toward deployment of high-temperature polymer electrolyte membrane fuel cells (HT-PEMFCs) in our daily lives, multiple research efforts have been dedicated to develop high-performance phosphate-doped polymer electrolytes. Recently, ion-pair coordinated polymers have garnered attention for their high stability and proton conductivity. However, a comprehensive understanding of how proton transport properties are modified by the functional groups present in these polymers is still lacking. In this study, we employ molecular dynamics (MD) simulations to investigate the impact of different functional group types and conversion ratios on conductivity. We find that Grotthuss-type hopping transport predominantly governs the overall conductivity, surpassing vehicular transport by factors of 100–1000. As conductivity scales with proton concentration, we observe that less-bulky functional groups offer advantages by minimizing the volume expansion associated with increased conversion ratios. Additionally, we show that a strong ion-pair interaction between the cationic functional group and the phosphate anion disrupts the suitable intermolecular orientations required for efficient proton hopping between phosphate and phosphoric acid molecules, thereby diminishing the proton conductivity. Our study underscores the importance of optimizing the strength of ion-pair interactions to balance stability and proton conductivity, thus paving the way for the development of ion-pair coordinated polymer electrolytes with improved performance.

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Poster Presentation : **POLY.P-37**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

The Effect of Free Volume Content in Poly(bismaleimide-alt-styrene) Network via Control of Oligomeric BMI Units for Low Dielectric Properties.

Leekyung Kim, Jinsoo Kim[1,*], Jong Chan Won[1,*], Jongmin Park[2,*]

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The dielectric property of the polymeric materials originated from the dipole moment of the chemical bonding and the molar density of the matrix. The relationship between chemical structure and dielectric property is known to be represented by the Clausis-Mossotti equation. According to the equation, the dielectric constant of polymer materials is proportional to molar polarizability, suggesting that the dielectric constant becomes lower as the increase of free volume between the polymer chains. Here, we designed a polymer network containing free volume as a cross-linking system with oligomeric bismaleimide (BMI). The robust aromatic BMI allows us to arrest the free volume between the aromatic building units by forming the aromatic polymer network. Our BMI resins have improved dielectric properties (Dk:2.76, Df:0.0029 at 10 GHz) compared to the reported BMI resins (Dk:3.0-3.8, Df:0.005-0.02 at 10 MHz). By doing so, we present a method to control the free volume of polymer networks by varying three parameters, including BMI molar mass, as a factor to obtain the desired dielectric properties. The invented low-dielectric BMI is expected to be useful in the field of 5G-level communication to achieve a high-quality communication system at a high-frequency regime (> 10 GHz).

Poster Presentation : **POLY.P-38**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Design of Ion-conducting Polyimide as the Protection Layer for Aqueous Zinc-ion Battery with Enhanced Cycling Performance

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[1]*Center for Chemical Materias, Korea Research Institute of Chemical Technology, Korea*

Ion-conducting polyimide is the class of high-performance polymer material containing the polar and charged functional groups that are facilitated to conduct the ion through the polymer matrix. This functional polymer has been utilized in battery applications as the polymeric electrolyte, electrodes, and binder material because of its thermal/mechanical/chemical stability. The special use in the next-generation battery application is the protection layer for the metal anode material. This protection layer helps to suppress the formation of dendrites by protecting random deposition ions on the anode surface, which is essential to extend the life cycle of the battery. By adopting a zinc-ion battery as the model system, we designed an ion-conducting polyimide as a protecting layer by introducing carbonyl and ether groups, which control Zn2+ ion diffusion. We found that the random nucleation on the anode surface differed by the embedded functional groups in the polyimide, resulting in variation in the life cycle performance of the battery. Our discussion about the ion-conducting property and chemical structure of the polyimide will suggest the plausible functional moiety to design high-performance functional polyimides.

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Poster Presentation : **POLY.P-39**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Li-conducting Functional Nanoporous Polymer Membrane with 10 nm-sized Channel to Achieve Long-cycling Lithium Metal Batteries

<u>Taeseok Oh</u>, Hye Ryung Byon*, Myungeun Seo*

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

Lithium metal batteries (LMBs) are gaining a lot of attention and demand thanks to their high energy density. To commercialize lithium metal batteries, the dendrite formation causing safety issues and dead Li formation must be resolved. However, commercial separators such as Celgard show difficulty in suppressing dendrite formation during the charge/discharge process. A separator to be used in LMB should have various properties; Solvent affinity and ionic conductivity, mechanical strength, pore size on the ~10 nm scale, chemical stability, etc. It was difficult to secure both conductivity and transport control by modifying the existing separation membrane to introduce macropores and micropores. Here, we propose a functional mesoporous functional polymer membrane incorporating a methodology of pore size control. The synthesized polymer has three-dimensional continuous pores through polymerization-induced microphase separation, and the size of the pores can be controlled by adjusting the molecular weight of the sacrificial block. Additionally, by introducing a negative charge to the pore surface, the conductivity of lithium ions can be increased and side reactions on the surface of the lithium electrode through negative ions can be suppressed. Through this study, we synthesize a separator that suppresses dendrites by observing and optimizing changes in lithium-ion conductivity and transference number according to pore size. To the best of our knowledge, this study is the only study to control pore size in LMB separator research.

Poster Presentation : **POLY.P-40**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Accessing to kinetically captured ordered morphologies via polymerization-induced microphase separation with incorporation of high χ monomers

Seungjin Ha, **Myungeun Seo**[*]

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

Polymerization-induced microphase separation (PIMS) serves as a versatile technique for creating 3D bicontinuous nanostructures. The selective etching of a specific domain enables the production of 3D bicontinuous nanoporous materials possessing significant potential for applications in separation, catalyst support, adsorption, and more. While the properties of nanoporous materials are closely related to the morphologies, such as lamella, cylinder, and gyroid, the kinetic trapping of phases during morphology development hinders the attainment of ordered structures. To address this kinetic challenge and achieve an ordered structure, we introduced a high χ monomer to expedite phase separation. Reversible addition–fragmentation chain transfer (RAFT) polymerization was employed for synthesizing block copolymers, with or without the high χ monomer. Depending on the presence of the high χ monomer, we observed kinetically trapped ordered morphologies, such as cylinders, lamellae, or gyroid.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Antagonistic Chiral Communication between Supramolecular Helices in Hierarchical Self-Assembly

Jun Su Kang, Kangseok Kim[1], Myungeun Seo[*]

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

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

The vital functions in lives are ingeniously governed by biological superstructures, such as superhelices of DNA, coiled-coil helix bundle proteins, and protein-DNA hybrid superstructures. These structures rely on a series of transfer and amplification of chirality between their components during the hierarchical self-assembly process. While many studies have reported the chiral interactions between the molecular level leading to helical assemblies and polymeric chains in self-assembling systems, few reports have highlighted hierarchical chiral communication between helical supramolecular components beyond the molecular level. Here, we explore the emergence of supramolecular chirality derived from chiral communication between helical structures. We employed hierarchical self-assembly of chiral and achiral triarylamine (TAA) derivatives as a model system. We will discuss temperature-dependent chiral amplification of their co-assemblies leading to the formation and deformation of TAA superstructures. This work will provide a clue as to how helical chirality can be transferred and amplified to higher levels of architecture from the molecular scale.

Poster Presentation : **POLY.P-42**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Effect of Polymer Architecture on Stabilization of Oil-Water Interface

Muniyappan Boominathan, Myungeun Seo[1,*]

Korea Advanced Institute of Science and Technology, India

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

An amphiphilic copolymer containing hydrophilic and hydrophobic segments can stabilize the water-oil interface by reducing interfacial tension. A classic example is a diblock copolymer such as polystyrene-b-poly(ethylene oxide) (PS-b-PEO), which is preferentially adsorbed at the oil-water interface with the partitioning of the PS and PEO blocks into the corresponding phases. In this work, to evaluate the architectural effect on interfacial stability, a synthetic methodology needs to be developed firsthand to access different architectures such as block, star, and graft from identical building blocks with minimal modifications. We evaluated the interfacial activity of the synthesized copolymers at the water-toluene interface and examined the stability of the oil-in-water emulsions containing toluene droplets and high internal phase emulsions (HIPEs) with a thin toluene continuous phase, generated by using the copolymers as emulsifiers.

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Poster Presentation : **POLY.P-43**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Understanding and Enhancing Optical Response through Positional Variation of Diacetylene Groups in Supramolecular Chirality

Kangseok Kim, Jun Su Kang, Myungeun Seo*

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Biomolecules like amino acids and proteins, which show a preference for a specific direction, exhibit more efficient and systematic characteristics compared to man-made polymers. There are ongoing efforts to uncover the origins of homochirality in such biomolecules. A significant portion of this research is focused on self-assembled supramolecular structures. These structures exhibit supramolecular chirality, which is dynamic and changes in response to external stimuli. This unique cooperative attribute allows for the amplification of circular dichroism (CD) signals. In particular, we have managed to manipulate the handedness of structures using diacetylene-containing triphenylamine (DA-TPA) and circularly polarized light (CPL), revealing the mechanisms behind this chiral transfer process.1,2 However, our understanding of the relative positioning and connectivity between the TPA core and the diacetylene group is still limited. In this study, we aim to pinpoint the factors that cause changes in the self-assembly process due to the positional variation of diacetylene groups, and present molecules that trigger an enhanced optical response.

Poster Presentation : **POLY.P-44**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Crystallization-Driven Self-Assembly of 2D Platelets to Form 3D Crystals by Controlling the Stereochemical Sequences of PLLA/PDLA-PEG Block Copolymers

Jae Hak Lee, Kyoung Taek Kim[1,*]

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

Discrete polymer, which has precisely defined molecular weight, molecular weight distribution, and sequence, has been of great interest as it can control the morphology of nanostructures due to its specifically defined chemical and physical properties. Crystallization-Driven Self-Assembly (CDSA) is one of the promising area which can control the conformation of self-assembled structure, as the crystallizable core-forming block requires a precise control. Interestingly, although flat 2D platelets are usually obtained from CDSA, we observed that 3D crystals can be formed by stacking the pre-formed 2D platelets. We assume that this uncommon phenomenon originates from the extra D-lactic acids units which allows the stacking of multiple platelets. We believe that this result can open the possibility of huge diversity of applications for future advanced polymeric materials.

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Poster Presentation : **POLY.P-45**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Induced Chain Folding of Precise Poly(l-lactic acid) and Their Sequence-Specific Degradation

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Seoul National University, Korea
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Poly(L-lactic acid) (PLLA) is a promising biodegradable polymer used in various applications, however, its degradation rate is notoriously slow. While high molecular weight is essential for improving the physical properties of degradable polymers, it significantly blocks their degradability due to conflicting requirements. For example, PLLAs are hydrolyzable, but enzymatic degradation becomes challenging at high molecular weights.To address this, we first designed the sequence-defined PLLA derivatives which have "breaking points" at specific intervals of LLA units to accelerate degradation with retained physical properties. Intentionally inducing folding in polymers at specific intervals enables them to maintain favorable properties without disrupting crystallite formation. According to our previous reports, we discovered that PLLAs fold at approximately 32 repeating units to form crystallites in the core of PLLA crystals. We envisioned that implementing DIC-mediated step-growth polymerization introduce breaking points along the PLLA backbone at specific intervals of LLA units (e.g. 32, 48 and 64 units). Positioned at the apex of the PLLA crystal, the breaking point is designed not to interfere with crystallite formation, thus preserving the polymer's physical properties. Upon exposure to certain conditions, the polymer can undergo intramolecular cyclization, leading to depolymerization and accelerated environmental degradation. This approach offers a controlled and selective means to trigger degradation in high molecular-weight polymers while maintaining their characteristics.

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Poster Presentation : **POLY.P-46**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Amorphous porous polymers based on heteroatom-containing spacers for water purification

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Fresh water is crucial for the fundamental sustainability of human societies worldwide. Amorphous porous polymers have emerged as promising materials for water purification due to their facile guest diffusion and excellent adsorption capabilities. In this study, we compared and analyzed the impact of heteroatom-containing spacers integrated into the structure of amorphous polymers on the adsorption of organic contaminants in water. Specifically, we varied the structure of heteroatom-bearing aromatic spacers in amorphous covalent organic framework (COF) structures and linear polymer structures, and compared their adsorption behaviors. We revealed that rational molecular design enables the ultrarapid adsorption of organic micropollutants with high removal efficiency (~99.9 % in 10 seconds) and achieves a record kobs (21.9 g mg-1 min-1). This study provides novel insights for the molecular engineering design of amorphous polymer materials with a focus on guest affinity in water purification.

Poster Presentation : **POLY.P-47**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

Enhancement of thermal properties of phthalonitrile networks controlled by curing agent

Eunkyung Jeon

Agency for Defense Development, Korea

High performance polymers with excellent thermal properties have attracted a lot of attention in the aerospace and defense industries. We synthesized phthalonitrile networs with high thermal stability using phthalonitrile resin and diamine as a curing agent. The curing process was optimized by controlling the type and concentration of diamine, and the network structure with high crosslinking density was obtained. The phthalonitrile network exhibits high glass transition temperature at approximately 450 degree C and excellent thermal oxidation stability with 95% weight retention in the rage of 500 to 550 degree C

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Poster Presentation : **POLY.P-48**
Polymer Chemistry
Exhibition Hall 2 THU 11:00~13:00

A novel fluorescent dye for staining microplastics with aggregation-induced emission (AIE) properties

Soo Seong Lee, Cheal Kim*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Microplastics are particularly concerning as they can pose lethal threats to marine environments and organisms. Thus, it is important to detect microplastics in the aquatic ecosystem. A novel fluorescent dye SS was synthesized at a low cost for detection of microplastics. SS showed novel aggregation-induced emission (AIE) properties, which was investigated by fluorescence spectroscopy. Moreover, strong fluorescence of SS in solid state rendered it suitable for microplastic staining. The microplastics staining using SS was conducted in 100% water to apply AIE properties. SS successfully stained five microplastics (PE, PET, PS, PU, and PVC), resulting in intense green fluorescence images. This demonstrated strong binding affinity of SS to microplastics. Our findings highlight the potential of SS as a powerful tool for low-cost and efficient detection of microplastics in aquatic environments. This research was supported by Green Convergence Technology Specialized Graduate Program through the Korea Environmental Industry & Technology Institute(KEITI) funded by the Ministry of Environment(MOE).

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Sequential Esterification and Thiol-ene Click Reaction Mediated Orthogonal Functionalization into Single Side Chain via Post-Polymerization Modification

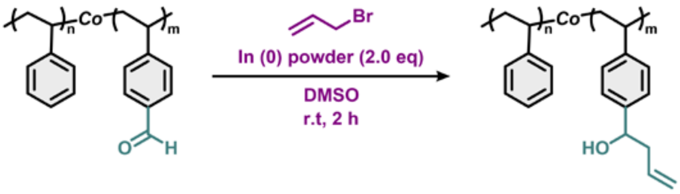
HyoWon Lee, Jeung Gon Kim[1,*]

Department of chemistry, Jeonbuk National University, Korea

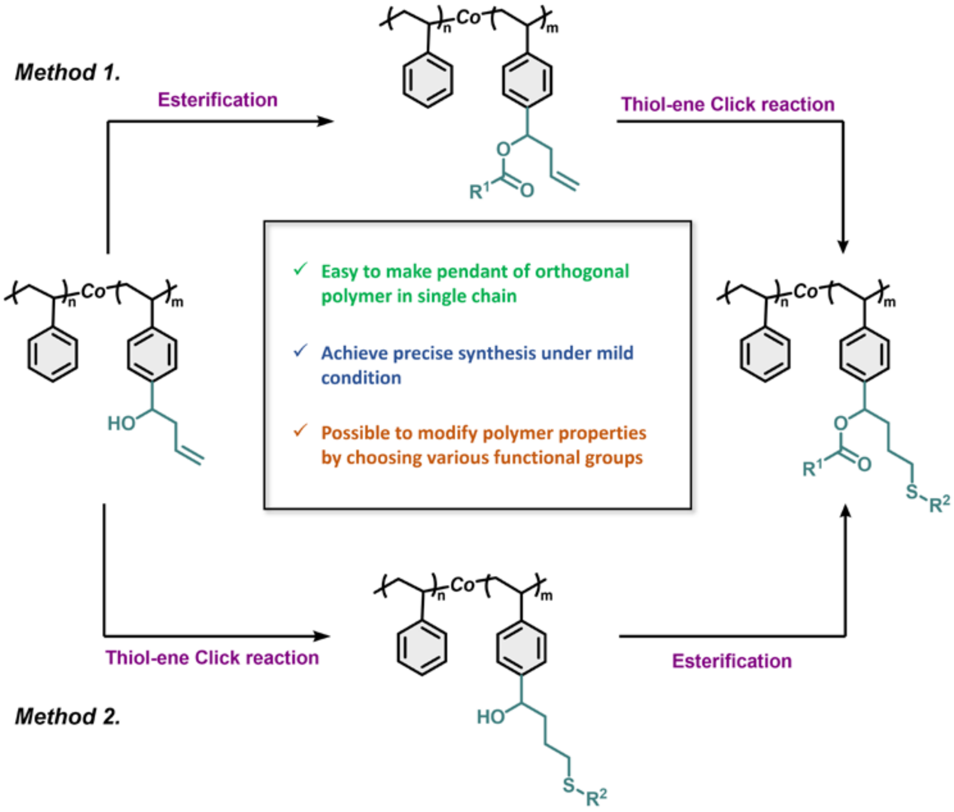
[1]*Department of Chemistry, Jeonbuk National University, Korea*

We describe the facile synthesis of orthogonal pendants through the highly reactive aldehyde polymer via post-polymerization modification (PPM) assisted Barbier-type allylation, utilizing harmless pure indium powder. The complex polymers were designed to enable the synthesis of highly efficient multifunctional polymers through sequential esterification and thiol-ene click reactions. All reactions were performed under mild conditions, and the proposed method is a novel technique to improve the diversity of polymer for applying to thermoreactive polymers and biomaterial polymers.

Post-Polymerization Modification: In(0)-mediated Barbier-type allylation



Orthogonal Post-Polymerization Modification: Esterification and Thiol-ene Click reaction



- ✓ Easy to make pendant of orthogonal polymer in single chain
- ✓ Achieve precise synthesis under mild condition
- ✓ Possible to modify polymer properties by choosing various functional groups

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Poster Presentation : **POLY.P-50**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

A staining agent for selective detection of microplastics

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[1]*Fine Chemistry, Seoul National University of Science & Technology, Korea*

A huge amount of microplastics (MPs) is currently drifting in the earth. They have the power to disrupt ecosystems and adversely impact on the growth of plants, animals, and even human health. Thus, it is important to monitor MPs pollution in the environment. A novel stain reagent Q was developed to monitor MPs. Q showed strong yellow fluorescence. Also, the solvatochromism of Q was investigated using fluorescence spectroscope in various solvent. Q showed highly selective detection of MPs over non-plastics under the fluorescence microscope. This research was supported by Green Convergence Technology Specialized Graduate Program through the Korea Environmental Industry & Technology Institute (KEITI) funded by the Ministry of Environment (MOE).

Poster Presentation : **POLY.P-51**

Polymer Chemistry

Exhibition Hall 2 THU 11:00~13:00

Designing Degradable Polymers from Tricycloalkenes via Complete Cascade Metathesis Polymerization

Tae-Lim Choi*, Yongkang Yang[1]

Division of Chemistry, Seoul National University, Korea

[1]*Department of Materials, ETH Zurich, Switzerland*

Cascade metathesis polymerization has been developed as a promising method to synthesize complex but well-defined polymers from monomers containing multiple reactive functional groups. However, this approach has been limited to the monomers involving simple alkene/alkyne moieties or produced mainly non-degradable polymers. In this study, we demonstrate a complete cascade ring-opening/ring-closing metathesis polymerization (RORCMP) using various tricycloalkenes and two strategies for the efficient degradation. Through rational design of tricycloalkene monomers, the structure and reactivity relationship was explored. For example, tricycloalkenes with trans configuration in the central ring enabled faster and better selective cascade RORCMP than the corresponding cis isomers. Also, a 4-substituted cyclopentene moiety in the monomers significantly enhanced the overall cascade RORCMP performance, with the maximum turnover number (TON) reaching almost 10,000 and molecular weight up to 170 kg/mol using an amide-containing monomer. Furthermore, we achieved one-shot cascade multiple olefin metathesis polymerization using tricycloalkenes and a diacrylate, to produce new highly A,B-alternating copolymers with full degradability. Lastly, we successfully designed xylose-based tricycloalkenes to give well-defined polymers that underwent ultra-fast and complete degradation under mild conditions.

Poster Presentation : **IND.P-52**
Industrial Chemistry
Exhibition Hall 2 THU 11:00~13:00

Synthesis of Noble Anti-PVY Pesticide Candidates

Seok Joon Lee*, **Sangtae Oh**[1]

Department of Pharmacology, Catholic Kwandong University, Korea
[1]*Department of Basic Sciences, Catholic Kwandong University, Korea*

Viral infections, similar to the Covid pandemic, often cause significant harm to humanity. Plants, too, suffer damage from various viruses, and the impact of viruses on food resources can pose a major threat to humanity. Among various plant resources, potatoes are a very important food source. The most damaging virus to plants is PVY, yet research on pesticides to treat it has not been extensively conducted. Our laboratory has been synthesizing and screening numerous compounds to develop new antiviral treatments. In this process, we have discovered a library of compounds that effectively suppress PVY. In this presentation, we intend to discuss the synthesis process of these substances.

Poster Presentation : **IND.P-53**

Industrial Chemistry

Exhibition Hall 2 THU 11:00~13:00

Combination Therapy for the Suppression of PVY

Seok Joon Lee*, **Sangtae Oh**[1]

Department of Pharmacology, Catholic Kwandong University, Korea

[1]*Department of Basic Sciences, Catholic Kwandong University, Korea*

Various methods have been developed to suppress viral infections. Typically, pharmacotherapy and vaccines are the most effective methods, but no method is perfect. Especially since vaccines cannot be used for plant virus infections, the development of various drugs is essential. Although recent studies on plant virus infections have been conducted, they have not achieved satisfactory results. In this study, we attempted a combination therapy using two or more drugs to enhance the efficacy of the drugs. In this study, we intend to present the results of co-administration of a drug effective against the PVY virus and a candidate substance developed by our research team.

Poster Presentation : **IND.P-54**

Industrial Chemistry

Exhibition Hall 2 THU 11:00~13:00

Homebuilt solid-state NMR probes for analysis of specific materials

Minseon Kim, Yongae Kim[*]

Department of Chemistry, Hankuk University of Foreign Studies, Korea

The solid-state NMR has the advantage of being able to measure samples in various sample states, for example, crystalline materials, gel-states materials and amorphous powders. Most materials with those state can be found in polymers, liquid crystals and biopolymers. These substances can be measured with commercialized NMR systems or commonly used probes, but probes can be manufactured and used according to specific research purposes or sample characteristics. For this reason, homebuilt solid-state NMR probes have advantages of being able to have a shape and function that suits the purpose of the experiment and being manufactured at a low cost. In this laboratory, we were designed and manufactured solid-state NMR probes for various samples according to research purposes. In particular, in the case of biological samples such as lipid bilayer or bicelle containing membrane proteins, high-efficiency and high-function probes are required, so it is necessary to manufacture probes suitable for this purpose. Here, we introduce a variety of homebuilt solid-state NMR probes, including the homebuilt 400 MHz narrow bore (NB) and wide bore (WB) ^{1}H-^{15}N solid-state NMR probes.

Poster Presentation : **INOR.P-1**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Phenyl-Olefin Dimerization in Metal-Organic Frameworks incorporating Bifunctional Olefin Ligands

Kyunghye Ju, TaeHun Kim, In-Hyeok Park*

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

Photoreactive isoreticular Zn(II) metal-organic frameworks (MOFs) with **pcu** topology were synthesized via solvothermal reaction employing zinc nitrate hexahydrate, *trans*-2-(4-pyridyl)-4-vinylbenzoic acid (Hpvba), and terephthalic acid derivatives (terephthalic acid (H_2bdc) and 2-aminoterephthalic acid (H_2NH_2bdc)). Single crystal X-ray diffraction analysis unveiled the crystal structures of pale yellow crystals of $[Zn_2(bdc)(pvba)_2]\cdot 2DMF$ (**1**) and pink crystals of $[Zn_2(NH_2bdc)(pvba)_2]\cdot 3DMF\cdot xH_2O$ (**2**) (DMF=dimethylformamide). MOFs **1** and **2** exhibited different degrees of interpenetrations (DOI) attributable to the dicarboxylate functionality. Calculations by PLATON yielded total potential solvent area volumes of 652.4 Å^3 (31.9%) for **1** and 3501.3 Å^3 (56.7%) for **2**, reflecting their distinct DOI. Under UV light, MOFs **1** and **2**, with 2-fold and 3-fold interpenetration, respectively, underwent partial [2+2] cycloaddition reaction, resulting in dimer formation from phenyl-olefin alignments. While the distance between the olefin-olefin bonds of the pvba ligands aligned by interpenetration remained photo-inert, the distance between the phenyl-olefin bonds fulfilled Schmidt's criteria for photoreactivity. Confirmation of phenyl-olefin cycloaddition dimerization in **1** and **2** was attained through ^{1}H nuclear magnetic resonance analysis (NMR). Further explanation will be provided in the poster presentation.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Spatial Distribution Control of Building Blocks in Multivariate Metal-Organic Framework with Anisotropic 3D Structure

Seonghwan Lee, Myoung Soo Lah*

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

Post-synthetic exchange serves as a potent technique to craft multivariate metal−organic frameworks (MOFs). These MOFs outperform in properties beyond the mere fusion of individual components. The post-synthetic ligand exchange (PLE) process in anisotropic 3D MOFs, which have pillared 2D layers, can cause a 1D contraction of the framework structure. This process can be effectively regulated by manipulating the temperature. At lower temperatures, the mixed building blocks form a microstructural MOF, which is homogeneous with a uniform distribution. However, as the temperature increases, the distribution transforms. It becomes heterogeneous, featuring a 2D concentric distribution of mixed building blocks. The reverse PLE process triggers a 1D expansion of the framework structure. This can create a heterogeneous microstructural MOF characterized by a 1D sandwiched distribution due to varying exchange kinetics between the layers. However, as temperatures increase, this layer selectivity diminishes, leading to a change of the building block distribution in the MOF structure. It evolves into another form of a heterogeneous microstructural MOF, this time exhibiting a 3D core−shell distribution.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Regulation of MMP-2/9 by Flavonoids

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For many decades, extensive research efforts have been dedicated to uncovering novel treatments for cancers and Alzheimer's disease (AD). Matrix metalloproteinases (MMPs) perform vital functions in several pathological processes, specifically, MMP-2 and MMP-9, have emerged as promising targets in cancer research due to their crucial roles in cancer development. Since they are involved in tumor cell invasion, angiogenesis, immune evasion, and metastasis, the enzymes could be considered as significant factors in cancer pathogenesis. Recent studies of natural products suggest that plants are essential sources that exhibit anticancer activities through regulating MMP and tissue inhibitor of metalloprotease (TIMP). Within the numerous compounds from vegetables and fruits have shown promising inhibitors against matrix metalloproteinases, particularly flavonoids. Flavonoids are one of the main groups of polyphenols found in fruits and vegetables which contain antioxidant properties and can help eliminating toxins from our body. Therefore, the primary objective of this study is to explore the pathogenic mechanisms by investigating the connection between MMP-2/9 and natural products. Through biological and biochemical experiments, we investigated how certain flavonoids influence the expression and activity of MMP-2/9. The selected flavonoids in this study have the potential to affect (i) the activity of MMP-2/9 possibly located at the active site, (ii) cytotoxic potential, and (iii) the expression of MMP-2/9, ERK-1/2, and JNK-1/2. This study provides novel insights into how flavonoids regulate MMP-2/9. Moreover, it could contribute to the development of another library of natural products for human diseases, including cancers and AD.

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

Inorganic Chemistry

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The Regulating Ability of Metal Ions Toward Matrix Metalloproteinases

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Recent days, the most troublesome diseases are cancer and neurodegenerative diseases (ND), including Alzheimer’s disease and Parkinson’s disease. Medical scientists have tried to develop an effective strategy to treat these diseases. Matrix metalloproteinase (MMP), particularly MMP-2 and MMP-9 play an important role in the pathogenesis of various cancers and ND. Therefore, many studies have been conducted to find out how to regulate its expression and activity. In this study, we focused on the interrelations between metal ions essential for our life [e.g., Na(I), Mg(II), Ca(II), Fe(III), and Al(III)] and MMP-2/9. Moreover, this study also aims to understand the pathogenic mechanisms based on the relationship between MMP-2/9 and metal ions. Through multiple biological and biochemical experiments, we examined the impact of various metal ions on the expression and activity of MMP-2/9 in cancer cells and neuronal cells. The activity of MMP-2 is suppressed when the concentration of divalent metal ion and trivalent metal ion is high, while monovalent metal ions could not affect the action of MMP-2. However, in case of MMP-9, none of metal ions significantly reduced the activity. This study could provide new insights into the regulation of MMP-2/9 based on its interaction with the fundamental metal ions for our life and contribute to the understand the pathology of cancers and ND.

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

Inorganic Chemistry

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Synthesis, Characterization and Evaluation of Metal Complexes Supported by (*E*)-2-Morpholino-*N*-(thiophen-2-ylmethylene)ethanamine as Multifunctional Biological Agents Including Docking Studies

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Transition metal complexes for treating diverse diseases have recently under the spotlight. Particularly, complexes supported with Schiff base ligands comprising heterocyclic moieties have gained attention due to their ability to bind multiple biological targets. Herein we used the thiophene-derived Schiff base ligand, (*E*)-2-Morpholino-*N*-(thiohen-2-ylmethylene)ethanamine for furnishing M(II) complexes, [TEM(M)X_2] (M = Co, Cu, Zn; X = Cl; M = Cd, X = Br) with the aim to be used an effective, versatile and valuable biological agents. Structural characterization of complexes revealed distorted tetrahedral geometry around the M(II) center. *In vitro* investigation of the synthesized ligand and its M(II) complexes showed that complexes exhibited superior bactericidal, fungicidal, and leishmanicidal activities. A preliminary study of human colorectal cancer (HCT), hepatic cancer (HepG2), and breast cancer (MCF-7) cell lines showed marked anticancer activities of these complexes. The synthesized complexes also exhibited a significant inhibitory effect on urease, with IC_{50} values in the range of 3.9–19.9 µM. In addition, the docking results were consistent with the experimental results.

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Poster Presentation : **INOR.P-6**

Inorganic Chemistry

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Addition Polymerization Using Precatalyst Pd(II) Complex and Cocatalyst Borate Salt toward Various Cyclic Olefins

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Since palladium complex is an active precatalyst for the addition polymerization, we used a ligand, namely 1-(naphthalen-2-ylmethyl)piperidine (K25C), and a co-catalyst, *N*,*N*-Dimethylanilinium Tetrakis(pentafluorophenyl)borate (Borate), in conjunction with palladium(II) acetate [$Pd(OAc)_2$] for the *in-situ* addition polymerization of various cyclic olefins such as bicyclo[2.2.1]hept-2-ene (NB), 5-butylbicyclo[2.2.1]hept-2-ene (BuNB), methyl bicyclo[2.2.1]hept-5-ene-2-carboxylate (MeNB) and bicyclo[2.2.1]hept-5-ene-2-methanol (AAcNB). The experimental results demonstrated that the catalytic system maintained high conversion for NB with 98.5%, 99.1%, and 98.6%, regardless of the temperature conditions (0°C, 25°C, and 40°C). Variations in the catalyst:borate:monomer ratio (1:2:1000, 1:2:5000 and 1:2:10000) showed a decreasing conversion trend with increasing ratios (98.2%, 78.6%, and 41.8%). However, when using toluene as a solvent instead of chlorobenzene at 60°C, 80°C, and 100°C, the result revealed a reduced conversion with higher temperatures. Exploration of alternative monomers at 25°C with a 1:2:1000 ratio demonstrated a superior conversion for BuNB (91.3% exo, 57.1% endo), compared MeNB (1.6% exo, 1.3% endo), and AAcNB (11.5% exo, 3.2% endo). We also employed our catalytic system for co-polymerization of NB with BuNB, MeNB and AAcNB.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Biomineralization of Nickel hydroxides using Silk Fibroin for Energy Storage Applications

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Biomineralization is an effective technique for creating hierarchical structures with the controlled formation of specific crystal structures regulated by biomacromolecules. Particularly, Silk fibroin derived from cocoons has received attention in diverse applications. The integration of biomolecules with inorganic materials has received significant research interest and powerful strategies for obtaining highly promising materials for energy storage. In this study, we synthesized biomineralized Ni(OH)2 using silk fibroin as a biomolecule via a biomineralization approach. Furthermore, we optimized the tunable morphologies of biomineralized Ni(OH)2 by varying the silk fibroin, Ni2+ concentration, and various solvents. The resultant biomineralized Ni(OH)2 electrode material exhibits better charge storage performance, rate capability, and cyclic stability. This study provides a new perspective on the synthetic approach for obtaining bio-templated inorganic materials with energy storage properties. Moreover, these hybrid materials can be explored in various applications such as biosensors, bioanalytical devices, and industrial biocatalyst fields.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Acid-triggered colorimetric sensor embedded metal-organic framework for optical identification of acid gases

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In safety and emergency response, identifying hazardous gaseous acid chemicals are vital for effective evacuation and appropriate first aid protocols, yet current acid sensors hardly differentiate between acids. We propose a simple, on-site monitorable colorimetric acid gas decoder, MOF-808-EDTA-Cu, using a robust MOF-808 coupled to Cu-EDTA as a proton-triggered colorimetric decoder that translates the different anion components of corrosive acids into visible colors. The sensor exhibited a remarkable cyan-to-yellow color transition in response to low concentrations of HCl gas and demonstrated the ability to visually identify various acid gases (HF, HBr, and HI) based on distinct color changes. Furthermore, the MOF-based decoder's versatility extends to multi-metal ions increasing the range of detectable gases, leading to the development of a portable miniaturized sensor capable of visually identifying 6 different colorless acid gases in a single sensor domain, proving its versatility as a practical sensor capable of on-site 24-hour monitoring in real-world.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Induced Production of Naturally Non-Preferred Metal–Organic Frameworks and Their Detachment via Post-Mismatching

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Metal–organic frameworks (MOFs) tend to adopt a naturally preferred form with a thermodynamically and kinetically stable structure. Hence, constructing MOFs having naturally non-preferred structures is a challenging task. Herein, we report a method to produce naturally non-preferred MOFs. Our approach relies on the registry between the surface of the template and the cell lattice of a target MOF, which reduces the effort required to form naturally non-preferred MOFs. Inductively grown MOFs are purely isolated from the template via provoking a post-mismatch in their lattices and weakening the interfacial interaction between product and template.

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Poster Presentation : **INOR.P-10**
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Synthesis of Metal(0) Coordination Compounds via UV-Activated Reactions

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In the process of exploring the properties and energy conversion of materials, chemical reactions in response to light play a complex and central role. These chemical reactions play an essential contributing to the optimization of solar energy utilization and the stable storage of chemical energy. The present work focuses on the photoactivation reactions between compounds based on carbonyl. The synthesized solution contains not only hexane and pyrazine, but also group 6 metal (0) carbonyl. Notably, these compounds are inert to heat but engage in photochemical reactions under UV illumination. This leads to the formation of a novel coordination complex where pyrazine is attached in the positions vacated by carbonyl groups. Furthermore, UV exposure promotes color change in the solution. This research is anticipated to enhance exploration into innovative uses within the fields of chemistry and physics.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis and proton transport of coordination polymers based on nickel

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Coordination polymers are polymeric materials composed of central metal ions linked by ligands, allowing the formation of unique polymers with diverse properties and structures using various metals and ligands. Because of these characteristics, coordination polymers are utilized in various sectors such as sensors and energy storage devices. Additionally, within the structure of coordination polymers, proton transfer can occur through processes like hydrogen bonding, ion channels, or interactions with metal ions. However, past coordination polymers have encountered issues such as low proton transfer efficiency and structural instability, attributed to uncertainties in proton transfer pathways and complex internal structures. To tackle these difficulties, the proton transfer mechanisms within the specimens were indirectly witnessed and scrutinized via electrochemical impedance spectroscopy (EIS). Furthermore, understanding of the internal proton transfer pathways was achieved through X-ray diffraction analysis.

Poster Presentation : **INOR.P-12**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Gas content characterization for hydrogen-enriched slush liquified natural gas

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The escalation of global warming is chiefly attributed to the emission of greenhouse gases from internal combustion engines. Transitioning to greener alternatives, such as electric batteries or fuel cells, represents a strategic pivot. However, the economic burden of engine replacement across diverse sectors, including manufacturing and maritime industries, is considerable. A feasible approach entails maintaining existing engines while modifying the fuel composition. Herein, we introduce an innovative concept: hydrogen-enriched slush liquified natural gas (H_2-SLNG), a synergistic blend of hydrogen and methane in a semi-solid state that straddles the boundary between solid and liquid phases. This novel strategy is designed to diminish CO_2 emissions while maintaining compatibility with extant combustion engines. Our study aims to ascertain the ideal methane-hydrogen ratio through gas chromatography (GC) analysis, employing thermal conductivity detectors (TCD) to precisely quantify the gas compositions. This would shed light on the interaction between CO_2 and H_2, an important topic for inorganic chemistry and future studies on related development of eco-friendly catalysts, etc. This research embodies the fusion of inorganic chemistry principles with environmental engineering, leveraging the unique properties of inorganic gases to forge a sustainable path forward in fuel technology.

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Poster Presentation : **INOR.P-13**

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New tetrazole –thiolato Pd(II) and -Pt(II) complexes: synthesis, structures, and chemical properties

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Tetrazole-thiolato transition metal complexes formed from organic tetrazo-thiones have been continuously paid attention to the structural or various coordinative behaviors to the transition metal such as N or S-coordination, and N, S-coodination on the tetazole-thiolato moiety as well as their utility for inhibition of metal corrosion. In this study, as the alternating method of dipolar cycloaddition of transition metal azides with organic unsaturated compounds such as isothiocyanates or isocynaides, we here attempt new method for the formation of tetrazole-thiolato complexes from direct reactions using organic tetrazole-thiones toward late transition metal alkyl complexes or its zero-valent complexes. Compared to the previous tetrazole-thiolato formation, we expect that the direct reactions using organic tetrazole-thiones, 1-alkyl(or aryl)-1H-tetrazole-5(4H)-thiones {S=[CN_4H(R)](R = alkyl or aryl)} are facile and convenient way to afford various or selective Pd(II) or Pt(II) tetrazole-thiolates. We further examined small molecule insertion studies using organic isocyanides and investigate electrophile treatments to afford various organic tetrazole- sulfides into the isolated Pd(II) or Pt(II) tetrazole-thiolate.

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

Inorganic Chemistry

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Enhancement of Antibacterial Properties through Spatiotemporal Photo-Oxidation of Shape-Controlled Cu_2O Nanoparticles

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The global community recognizes antimicrobial resistance as a significant threat to public health. Recent research challenges previous assumptions, revealing that nanoscale antibacterial agents based on metals can be susceptible to resistance. Although the exact mechanism is not fully understood, it is clear that repeated exposure can lead to resistance, primarily due to limited antibacterial effectiveness. This study introduces two approaches to create a highly concentrated Cu^{2+} environment to enhance antibacterial efficacy. The first involves using Cu_2O nanoparticles to induce thermal convection, concentrating bacteria. The second utilizes light to break down nanoparticles, rapidly generating Cu^{2+} in regions with bacterial infestation. This experimental method demonstrates the effective elimination of confined microorganisms in a short time. Additionally, we suggest optimal morphological characteristics for Cu_2O nanoparticles to maximize effectiveness through controlled manipulation of facet junctions.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Uncovering Four-Electron Dioxygen Reduction Routes and Reactive Intermediates with Phosphorus-Ligand Redox Cooperative Catalysis

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The reduction of oxygen is essential in both biological processes and energy technologies. However, it is challenging due to the inert nature of oxygen and its complex mechanisms. In nature, high-spin transition metal complexes are used for this purpose, whereas main-group compounds, with their singlet state and limited redox capabilities, show less reactivity. We introduce a new phosphorus complex that can perform four-electron reduction of oxygen, facilitated by a distinctive cooperation between the phosphorus atom and the ligand. Through spectroscopic and computational analysis, we found that this cooperative reactivity is due to the specific electronic structure resulting from the planar geometry of the phosphorus complex. Mechanistic studies involving spectroscopic and kinetic experiments revealed the presence of phosphorus intermediates similar to those found in metalloenzymes. Our findings underscore the multi-electron reactivity of phosphorus compounds enabled by a carefully designed ligand platform with redox cooperativity. We expect that this research will expand the approaches for developing main-group catalytic reactions, particularly those involving small molecule fixation requiring multi-electron redox processes.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Exploring Enhanced Thermoelectric Properties Through Transition Metal Substitution in Zintl Phases: The $Ca_9Cd_{4.5-x}M_xSb_9$ (M = Zn and Cu) System

Junsu Lee, Tae-Soo You[*]

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Thermoelectric (TE) materials and devices have great potential to reduce energy crisis and losses by converting wasted heat from various heat sources and converting it into electricity based on the Seebeck effect. Thermoelectric performance is defined as the dimensionless figure-of-merit $ZT = \sigma S^2T/\kappa$ (σ: electrical conductivity, S: Seebeck coefficient, T: absolute temperature, κ: thermal conductivity). The Zintl phase is one of the candidates for TE applications among TE materials such as clathrates, skutterudites, half-heusler, and PbTe. This is because a high Seebeck coefficient is expected as a semiconducting property and low thermal conductivity due to the complex structure. Recently, the Zintl phases within the A_2CdSb_2 (A = Ca, Yb, Eu; Ca_2CdSb_2 or Yb_2CdSb_2-type) system have been studied to enhance TE properties through cation ratio regulation. Additionally, we investigate changes in thermoelectric properties through the substitution of the transition metal Cd^{2+} with the divalent cation Zn^{2+} and the monovalent cation Cu^{+}, respectively. However, the resultant structure from this transition metal substitution is not the anticipated $A_2Cd_{1-x}M_xSb_2$ (M = Zn and Cu; Ca_2CdSb_2 or Yb_2CdSb_2-type, but rather $A_9Cd_{4.5-x}M_xSb_9$ (M = Zn and Cu; $Ca_9Zn_{3.1}In_{0.9}Sb_9$-type)—a distinct structure compared to the previously established $A_9M_{4.5}Sb_9$ (A = Ca, Yb, Eu, Sr; M = Zn, Mn; $Ca_9Mn_4Bi_9$-type) structure. Interestingly, $Ca_9Cd_{4.5-x}Zn_xSb_9$ ($x \geq 2.25$) produces a $Ca_9Mn_4Bi_9$-type structure, and $Ca_9Cd_{4.5-x}Zn_xSb_9$ produces a $Ca_9Zn_{3.1}In_{0.9}Sb_9$-type structure. This phase change occurs depending on the size of the transition metal. A series of compounds in the $Ca_9Cd_{4.5-x}M_xSb_9$ (M = Zn and Cu) system were synthesized by metal flux reaction. Their crystal structures were characterized by both powder and single-crystal X-ray diffraction (PXRD and SXRD) experiments. To understand the electronic structure of the title compounds, a series of theoretical calculations using the tight-binding linear muffin-tin orbital (TB-LMTO) method was performed, and the resultant density of states (DOS), band structure, and electron localization function (ELF) analyses were thoroughly conducted. Physical properties including electrical conductivity, Seebeck coefficient, and thermal conductivity of the quaternary title compound the $Ca_9Cd_{4.5-x}M_xSb_9$ (M = Zn and Cu) were thoroughly examined.

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

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Controlling Thermoelectric Properties of the $BaZn_{2-x}Al_xSb_2$ System by Al-doping

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Thermoelectric (TE) materials are eco-friendly and sustainable solutions to global warming by converting wasted heat to electricity directly for producing industrial energy which can decrease greenhouse gas emissions. Among the various TE materials, the Zintl phase is the promising candidate due to its complicated crystal structure and intrinsic semiconducting properties. The ternary Zintl phase AM_2X_2-type (A = Ba, Sr, Eu, Yb, Ca; M = Zn, Cd; X = Sb) series have recently been thoroughly investigated, and these compounds displayed two classes of crystal structures: the $BaCu_2S_2$-type and the $CaAl_2Si_2$-type. In this work, the effect of Al doping on the Zn site for the ternary $BaZn_2Sb_2$ has been examined, and it resulted in producing the quaternary $BaZn_{2-x}Al_xSb_2$ system successfully. The title quaternary $BaZn_{2-x}Al_xSb_2$ ($0.16(2) \leq x \leq 0.53(2)$) series has been synthesized by the molten Pb-flux method, and their crystal structures were carefully characterized by the powder and single-crystal X-ray diffraction analyses (PXRD and SXRD). The resultant PXRD pattern indicated that the title compounds crystallized in the $BaCu_2S_2$-type phase. Based on the SXRD analyses, the density of compounds decreased as the component of Al increased. The site preference of the Al-dopant for the Zn2 site on the SXRD data was nicely explained by the QVAL according to the electronic-factor criterion. Energy Dispersive X-ray Spectroscopy analyses (EDS) also showed comparable results to the SXRD refinements. The density functional theory calculation (DFT) of a hypothetical model $BaZn_{1.5}Al_{0.5}Sb_2$ was performed to analyze the overall electronic structure of the title compounds as well as orbital distributions and chemical bonding. DOS, Band Structure, and -COHP analyses were thoroughly performed as well. By adding some Al-dopant at the Zn site, the effective mass of DOS increased near the Fermi level (E_F) in DOS curves,

and the complexity of graphs increased in Band Structure. In -COHP analysis, the antibonding characteristics of the Zn/Al-Sb bond at near Fermi level increase by the Al dopant. Electrical conductivity and Seebeck coefficient of title compounds were measured for appraisal of thermoelectric properties.

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

Inorganic Chemistry

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Novel Ligand Mold Design for Controlled Metal Growth on Gold Nanoparticles Using Linear-b-Bottlebrush Copolymers

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We present an novel approach utilizing ligands made from linear-b-bottlebrush copolymers (LBBCP) attached to gold nanoparticles (Au NPs) to serve as designated functional zones. The main objective is to develop a stiff nanoscale framework that can direct the formation of various metals. The arrangement of densely packed bottlebrush segments on the Au NPs' exterior is stabilized by the restricted room for their side chains, maintaining their placement. By altering the solvent environment, we successfully segregated the bottlebrush copolymers (BBCPs) into these dense areas. We were able to precisely control the segregation level by modifying the water to dimethylformamide (DMF) ratio. These compact Au-BBCP regions effectively prevent the entry of different metals, thus facilitating the generation of diverse BBCP patch shapes that serve as molds for silver (Ag) deposition on the Au NPs. As a result, we managed to create various bimetallic configurations, including uniform and textured core-shell designs, several isolated formations, and Janus configurations.

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

Inorganic Chemistry

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Improving Thermoelectric Property of the $BaZn_{2-x}Mg_xSb_2$ System by Using Earth-Abundant Mg

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60 percent of the energy used in industry is wasted and dissipated as heat energy. Thermoelectric materials convert this waste heat into electrical energy, improving energy efficiency. Among various thermoelectric materials, Zintl phases can be considered one of the best candidates. The AM_2X_2 system has been extensively investigated as a true-frame thermoelectric material. To investigate the effect of Mg substitution, we synthesized $BaZn_{2-x}Mg_xSb_2$ (x = 0.03, 0.06) series using the molten lead flux method. The synthesis produced bar-shaped crystals, which were successfully analyzed by Powder X-ray Diffraction (PXRD), Single-crystal X-ray Diffraction (SXRD), and Energy-dispersive X-ray spectroscopy (EDS) for various structures and elemental characteristics. XRD results show that Mg larger than Zn tends to increase the volume. The calculation using $BaZn_{1.5}Mg_{0.5}Sb_2$ to analyze the electron structure of the compound was performed using the tight-binding linear muffin-tin orbital (TB-LMTO) method, resulting in DOS curve, and band structure analysis. The inclusion of Mg in the DOS curve typically leads to a reduction in its magnitude, which in turn predicts a decrease in the Seebeck coefficient. The Mg-doped $BaZn_{1.5}Mg_{0.5}Sb_2$ showed an improvement in thermoelectric properties according to the electrical transport property measurement. Specifically, the $BaZn_{1.74(2)}Mg_{0.26}Sb_2$ sample exhibited the highest power factor recorded at 7.05 $\mu W/cmK^2$ at 748 K, indicating its efficiency in converting thermal energy into electrical power. Consequently, an increase in the *ZT* value can be expected for Mg-doped $BaZn_{1.74(2)}Mg_{0.26}Sb_2$.

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

Inorganic Chemistry

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Controlling the Oxidation state of Copper Nanostructures on Gold Nano-Electrode Ensembles Using Cyclovoltammetry

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Copper oxide (Cu_xO) is a highly promising material as an electrochemical catalyst. These compounds predominantly exist in the +1 or +2 oxidation state depending on the synthetic conditions. Furthermore, Cu_xO has the potential to form bimetallic alloys by combining with other metals, presenting possibilities as a tandem catalyst. In this study, we monitored the electrochemical phase transition of copper oxide at the single-particle level. The introduction of gold nanoelectrode ensembles effectively suppresses the dissolving process of electrochemically synthesized copper domains. The deposition and dissolving processes alternately conducted through cyclic voltammetry, clearly demonstrate differences in the presence of gold nanoparticles. We have expanded the mechanism study conducted to a large-scale system. Interestingly, the phase of the deposited copper domain is controlled depending on the presence of the heterogeneous nanoparticle support. The large-scale electrode synthesized on the gas diffusion layer can be applied to the carbon dioxide reduction reaction.

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

Inorganic Chemistry

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Introduction of BL2D-Supramolecular Crystallography Beamline at the Pohang Accelerator Laboratory

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Beam Operation Team, Pohang Accelerator Laboratory, Korea

The supramolecular crystallography beamline BL2D-SMC at the Pohang Light Source II (PLS-II) is a high-flux tunable-wavelength facility for the study of organic or inorganic materials by single crystal diffraction. The beamline supports various techniques for the structural analysis of crystalline materials, and allows the measurement of structural changes caused by the influence of external stimuli, e.g., variable temperature, diverse pressure, photo-excitation, and gas sorption. The beamline is located at the 2D bending magnet port in the 3 GeV storage ring of the Pohang Light Source II. Two mirrors (collimating and focusing) and a double-crystal monochromator (DCM) deliver 6.2×1011 photons each second to a 100 μm (horizontal) × 85 μm (vertical) full width at half maximum focal point in the end-station. A water-cooled DCM is designed to select energies between 8.3 keV and 20.7 keV and the energy or wavelength used in the system can be changed by the BL2DSMDC software. The end-station is equipped with a Rayonix MX225HS, Cryojet 5 and customized gas sorption apparatus. In this poster, we explain the status of BL2D-SMC beamline at Pohang Light Source II

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Tailoring Functional Groups with Different Polyaniline Derivatives for Fine-Tuning Water Harvesting

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Metal-organic frameworks (MOFs) are considered one of the most interesting porous materials because of their high specific surface area and tunable porous environment. However, MOFs are not utilized in the industrial fields yet because of their high cost and low stability. In this research, we remarkably increase the stability of Cu-paddlewheel MOF, HKUST-1, by post-synthetic methods incorporating aniline derivatives and oxidizing it in the MOFs. Cu-paddlewheel MOF catalyzes the chemical reaction of aniline to azobenzene and polyaniline. Because of the products for catalytic reaction, aniline-derivative treated HKUST-1 showed surprisingly increased hydrolytic and electrochemical stability. NMR, BET, FT-IR, and Raman are used to determine the reason for enhanced hydrolytic stability after the reaction with aniline derivates. Furthermore, the extremely increased hydrolytic stability can be used as a water-harvesting metal-organic framework. We also changed the functional group of aniline which can modify the chemical properties and find the appropriate one with the stability and water harvesting.

Poster Presentation : **INOR.P-23**
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2D conductive MOF and 3D high porous MOF hybrid-based room temperature chemiresistors with enhanced gas sensitivity

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A chemiresistor is a highly efficient gas sensor with low cost and high sensitivity. However, conventionally used metal oxide-based chemiresistors require temperatures as high as 150 °C or more for operation. Unlike them, 2D conductive MOFs exhibit superior chemiresistive performance at room temperature due to their intrinsic conductive structure resembling graphene with open metal sites. Nonetheless, general 2D MOFs have somewhat lower porosity than 3D MOFs due to structural limitations and limited crystallinity. This lower porosity reduces the contact area between the target gas and the MOF sensor, potentially limiting sensing performance. Our study introduces the method to maximize the gas sensing performance of a chemiresistor by hybridizing a highly porous 3D MOF with a high affinity for a specific gas with a 2D MOF in various way.

Poster Presentation : **INOR.P-24**
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Exhibition Hall 2 FRI 11:00~13:00

A redox active Co(III) aminyl radical species

Gyeongmin Park, Yunho Lee[1,*]

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

Stable metal bound organic radical generation is of our particular interest in our group since it is involved in various bond activation reactions as a key intermediate. To control the reactivity and redox activity, the reactive organic radical can be engaged in the primary coordination sphere of the transition metal ion. By sharing the spin-density between metal and organic radical, its character can be significantly altered. In particular, the pincer ligand can be employed to prepare 6-coordinate metal complexes, systematically, where the central N or C moiety can be located in both axial sites and directly interacted with the central metal ion to share the spin density. With this in mind, we have synthesized an N-heterocyclic carbene-containing bis(4-methyl-2-(3-methyl-imidazolium)phenyl)amine (CNC) pincer ligand and its cobalt complexes [Co(CNC)2](PF6)2 (1) and its reduced species [Co(CNC)2]PF6 (2). Both 6-coordinate cobalt complexes 1 and 2 reveal almost identical octahedral geometry although they are different each other by 1-electron. This is because the redox activity of 1 occurs not in the cobalt center but the amido moiety. According to the solid-state structural analysis and EPR spectroscopic data, the N–Co–N core of 1 reveals an aminyl radical character. Its DFT analysis also supports its assignment by showing that the major contribution in the SOMO is from two amido donors. Interestingly, compound 1 is a radical species but reveals unusual stability towards water and air, and it undergoes interesting redox activity coupled with acid/base chemistry, which will be discussed.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Ferroelectric materials affect Polar Proteins in Tumor Treating Fields

Juhyeong Cho, Daeha Seo[1,*]

Department of the Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Electric fields serve as one of the useful tools for researching various polar substances and ions within cells. Depending on their size and type, they can affect various components of the cell, particularly low-intensity alternating electric fields, known as Tumor Treating Fields (TTFields), have shown specific effects on proteins such as tubulin, which constitute microtubules and the mitotic spindle. Recent studies have shown that combining ferroelectric nanoparticles with TTFields can enhance the therapeutic effect, but the mechanism of action is still not clearly understood. In this study, we utilized tetragonal BaTiO3 (T-BTO) nanoparticles, known for their low cytotoxicity and high ferroelectricity, to explore the mechanism of interaction between ferroelectric nanoparticles and polar substances within cells in an alternating electric field. For this purpose, we synthesized multi-functionalized BaTiO3 nanoparticles (T-BTO@SiO2@BODIPY, Transferrin) and investigated the effects of combining them with TTFields on cellular behavior changes. The results confirmed that the introduction of nanoparticles was more effective in inhibiting cell proliferation compared to the use of TTFields alone. Through super-resolution radial fluctuation (SRRF) microscopy, we observed that the destruction of microtubules under TTFields was amplified in the presence of nanoparticles. While investigating the cause of microtubule destruction, we considered the possibility of reactive oxygen species (ROS) generation and steric hindrance, but our results did not support these hypotheses. Finally, we demonstrated a correlation between spontaneous polarization of nanoparticles and the results, thereby providing a new understanding of the mechanism behind the enhanced effect of TTFields treatment using ferroelectric nanoparticles. This study not only provides deep insights into the mechanism of enhancing the effect of TTFields with ferroelectric nanoparticles but also offers important implications for future nano-therapies and drug development.

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

Inorganic Chemistry

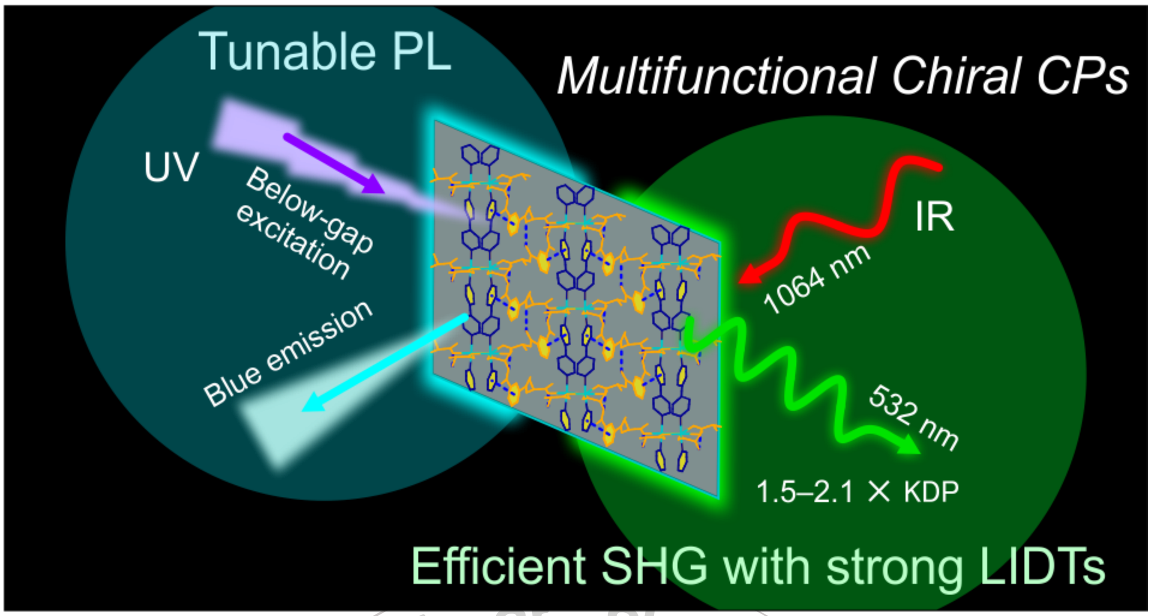
Exhibition Hall 2 FRI 11:00~13:00

Homochiral d^{10}-metal coordination polymers with tunable photoluminescence and efficient nonlinear optical properties

Jihyun Lee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Homochiral coordination polymers (HCPs), constructed through the coordination of metal cations and chiral ligands, offer a distinctive advantage in systematically designing noncentrosymmetric (NCS) structures. A new series of HCPs, $[M_2(SIAP)_2(bpy)_2]$ and $[M_2(RIAP)_2(bpy)_2]$ (M = Zn or Cd, SIAP or RIAP = (*S*,*S*)- or (*R*,*R*)-2,2'-(isophthaloylbis(azanediyl))di-propionic acid, bpy = 4,4'-bipyridine), has been synthesized using solvothermal reactions, assembling d^{10} metal cations, chiral dicarboxylic ligands, and π-conjugated bipyridyl ligands. These HCPs crystallize in the rare triclinic chiral space group, $P1$, forming three-dimensional structures driven by strong intermolecular interactions. With diverse functional groups in ligands, the HCPs exhibit efficient photoluminescence across a broad visible range, tunable by excitation wavelength. Additionally, the HCP compounds demonstrate efficient second-harmonic generation (SHG) with very high laser-induced damage thresholds. Notably, the compounds exhibit measurable contrast in the SHG response under circularly polarized excitation. This presentation will cover the synthesis, structure determination, and optical properties of these HCPs.


Tunable PL
Multifunctional Chiral CPs
UV
Below-gap excitation
Blue emission
IR
1064 nm
532 nm
1.5–2.1 × KDP
Efficient SHG with strong LIDTs

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Sterically Modulated Polar and Nonpolar Homochiral Perovskites

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Perovskite materials with polar structures, including piezoelectric sensors, nonvolatile storage devices, switches, and others, such as $MAPbX_3$ (MA: methyl ammonium, X: halides), have garnered significant interest across various fields owing to their remarkable ferroelectric properties. Discovering novel ferroelectric materials remains an ongoing challenge, as the crystal structures of solid-state materials should be noncentrosymmetric (NCS) polar structures. Many strategies for controlling centricity have been continuously proposed, but the majority of the products still tend to be centrosymmetric (CS) or NCS nonpolar structures due to the facile alignment of asymmetric units in an antiparallel manner. In this presentation, we propose a new strategy involving steric confinement modulations. We have successfully synthesized two hexagonal perovskites through solvothermal reactions. The crystal structures, determined using single crystal X-ray diffraction, indicate that both compounds belong to a chiral space group, attributed to the presence of chiral organic cations. The crystal structure of compound **1** was found to belong to the NCS nonpolar space group, $P2_12_12_1$, because the highly distorted constituting octahedral units align perfectly in an antiparallel manner. Conversely, the structure of compound **2** crystallizes in the NCS polar space group, $P2_1$, due to the tilted octahedra, a phenomenon attributed to the steric effect arising from the organic species. Details of the synthesis, crystal structures, and properties, along with density functional theory calculations, are also presented.

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

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Rapid purification of anisotropic gold nanobipyramids and directed secondary growth of silver nanoshells.

Sujin An, Jung-hoon Lee*

Department of Chemistry, Soonchunhyang University, Korea

Gold nanoparticles have unusual optical properties, unlike ordinary gold. This is mainly related to the phenomenon of surface plasmon resonance of nanoparticles. The surface plasmon resonance of gold particles is a phenomenon in which light waves travel around the surface to enhance their optical properties. In particular, the pointed ends of gold nanobipyramids enhance the plasmon resonance and simultaneously enhance the optical properties. Gold bipyramids provide photocatalytic and strong photonic effects, making them efficient in a variety of applications, including sensors and optoelectronic devices. This study aims to synthesise gold nanobipyramids, separate and purify them from other types of nanoparticles, and then grow them in two different directions. In the experiment of forming nanoshells on gold nanobipyramids, silver nanoshells on the core can be grown in the long-axis and short-axis directions by using different surfactants. The main advantage of growing the shell in the long and short axis directions is that it can further enhance the properties of light waves, which can improve the optical sensitivity, change the catalytic activity and improve the efficiency of chemical reactions on the surface of gold nanobipyramids. Previous studies have reported the synthesis of various shapes of nanoparticles using gold nanobipyramids as templates. However, there is currently insufficient literature on the precise synthesis of nanobipyramids grown in either the long or short axis direction at a small size of 50-100 nm. Therefore, the goal of this study is to synthesise gold nanobipyramids of a specific shape and then compare the synthesis yield with other gold nanoparticles to show reproducibility. This research is expected to open up new possibilities in the field of nanotechnology by understanding the morphological control and regrowth of nanoparticles.

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Poster Presentation : **INOR.P-29**

Inorganic Chemistry

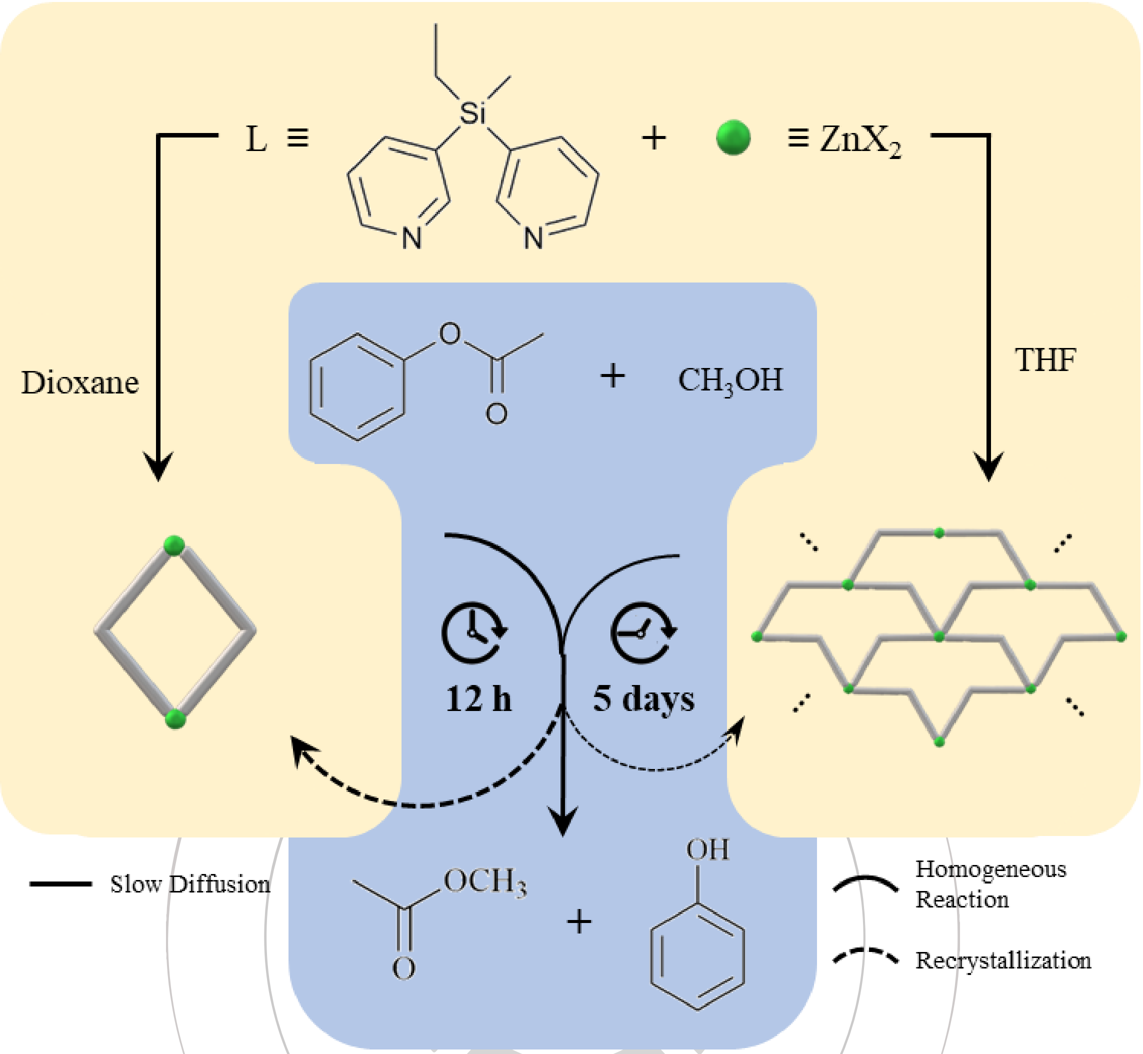
Exhibition Hall 2 FRI 11:00~13:00

High-Yield Recycling of Zn(II) Complexes as Catalysts: Structural Differences via Recrystallization Methods

Jihun Han, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly involving ZnX_2 (X^- = Cl^-, Br^-, I^-, NO_3^-) with ethyl(methyl)(3-pyridine)silane (L) as a bidentate N-donor ligand have been conducted. These interactions give rise to the formation of new discrete cyclodimeric rings and a 2D coordination compound. The complexes that consist of NO_3^- acts as a remarkable transesterification catalytic system which exhibits the added benefit of recyclability through homogeneous catalytic action.The outcome of the self-assembly process depends on the method chosen for recrystallization. Specifically, employing distinct recrystallization approaches yields either a high yield of discrete cyclodimeric rings or a comparatively low yield of the 2D coordination compound.


L ≡
Si
N
N
+
≡ ZnX$_2$
Dioxane
THF
O
O
+
CH$_3$OH
12 h
5 days
OCH$_3$
O
+
OH
Slow Diffusion
Homogeneous Reaction
Recrystallization

Poster Presentation : **INOR.P-30**

Inorganic Chemistry

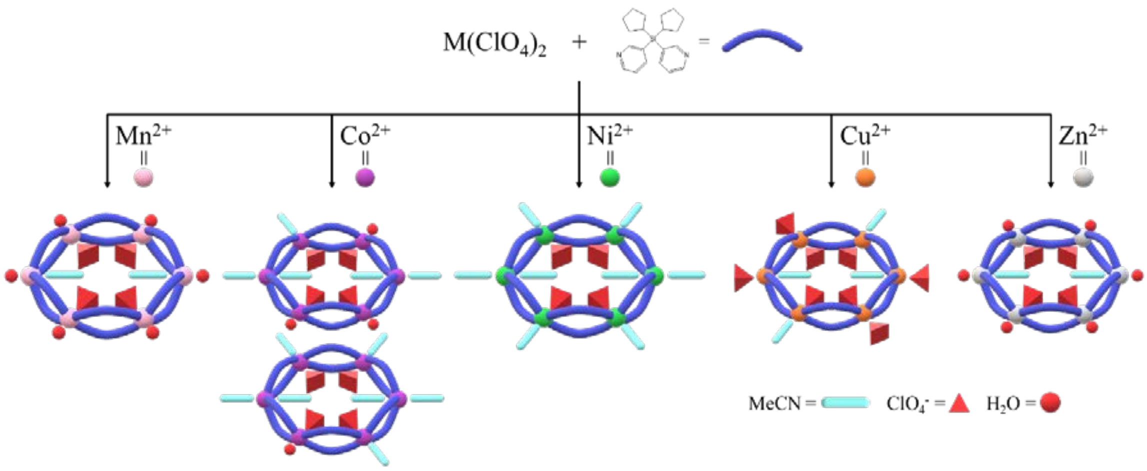
Exhibition Hall 2 FRI 11:00~13:00

Competitive bonding of perchlorate, water, and acetonitrile in M_6L_{12} double-stranded macrocycles mediated by metal(II) ions

Seonghyeon An, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

Self-assembly of $M(ClO_4)_2$ (M(II) = Mn(II), Co(II), Ni(II), Cu(II), and Zn(II)) with dicyclopentyldi(pyridine-3-yl)silane (L) as a donor in the same mixture of acetonitrile and toluene produces crystals consisting of M_6L_{12} double-stranded macrocycles. The geometry around the M(II) cations is a typical octahedral arrangement, but the metallamacrocycles outer axial coordination environment is sensitive to the M(II) cations. The conformation of the unique metallamacrocycles is informatively dependent on the nature of the coordination around the M(II) cations *via* subtle co-ligand competition among perchlorate anions, water, and acetonitrile. Both the coordinated acetonitriles and the solvate molecules of the crystals are removed at 170^{o}C, thereby transforming the crystals into new crystals of ring-opened products that return to their original form in the mixture of toluene and acetonitrile. Catalytic oxidation of 3,5-di-*tert*-butylcatechol using $[Cu_6(ClO_4)_8(CH_3CN)_4L_{12}]4ClO_4{\cdot}5C_7H_8$ is much faster than those using the ring-opened product, $[Cu(ClO_4)_2L_2]$, and the simple mixture of $Cu(ClO_4)_2$ + L.


M(ClO$_4$)$_2$ +
=
Mn^{2+}
Co^{2+}
Ni^{2+}
Cu^{2+}
Zn^{2+}
MeCN =
ClO$_4^-$ =
H$_2$O =

Poster Presentation : **INOR.P-31**

Inorganic Chemistry

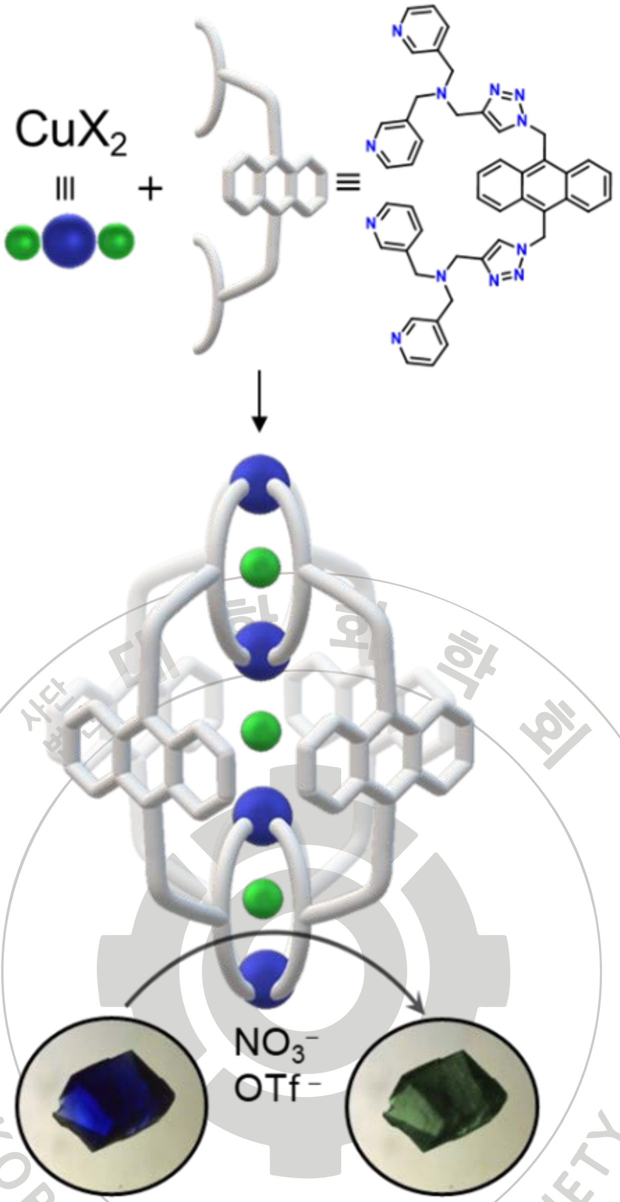
Exhibition Hall 2 FRI 11:00~13:00

Structural features of unprecedented 3X@Cu_4L_4 species: recognition of polyatomic anions

Hyo jeong Back, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of CuX_2 (X^- = Cl^- and Br^-) with *N*,*N*′-((1,1′-(anthracene-9,10-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis(methylene))bis(1-(pyridin-3-yl)-*N*-(pyridin-3-ylmethyl)methanamine) (L) as a C_2-symmetric multidentate *N*-donor gives rise to an unprecedented discrete propeller-type Cu_4L_4 architecture with a linear Cu-X-Cu-X-Cu-X-Cu arrangement, $[3Cl@Cu_4ClL_4(H_2O)]Cl_4$ and $[3Br@Cu_2L_4(H_2O)_2]Br_5$, respectively. For both species, the photoluminescence of the anthracenyl moiety significantly recognizes NO_3^- and $CF_3SO_3^-$ among various polyatomic anions including NO_3^-, $CF_3SO_3^-$, $Cr_2O_7^{2-}$, BF_4^-, PF_6^-, ClO_4^-, and I^-.


CuX$_2$
+
≡
N
NO$_3^-$
OTf$^-$

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Poster Presentation : **INOR.P-32**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis, crystal structure, and optical properties of a layered organic-inorganic hybrid material

Bo Young Kim, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

A novel layered organic-inorganic hybrid material has been synthesized using a slow evaporation method. We determined the crystal structure of the compound through single crystal X-ray diffraction. The compound crystallizes in the triclinic space group, *P*-1 (No. 2). Interestingly, the metal halide framework of the compound forms a unique layer, in which distorted octahedra are linked by face-, edge- and corner-sharing. Four-membered rings and ten-membered rings composed of $CdCl_6$ are observed. Organic cations are aligned through hydrogen bonding interactions between the N-H of the pyridine ring or amine and Cl in the $CdCl_6$. Ultraviolet-visible diffuse reflectance spectrum and photoluminescence measurements indicate that the compound possesses a large band gap of ca. 4.36 eV and exhibits blue-light emission. Moreover, the compound exhibits stability in air, water, and various organic solvents without undergoing decomposition. Thermogravimetric analysis reveals that the compound remains stable up to ca. 230°C.

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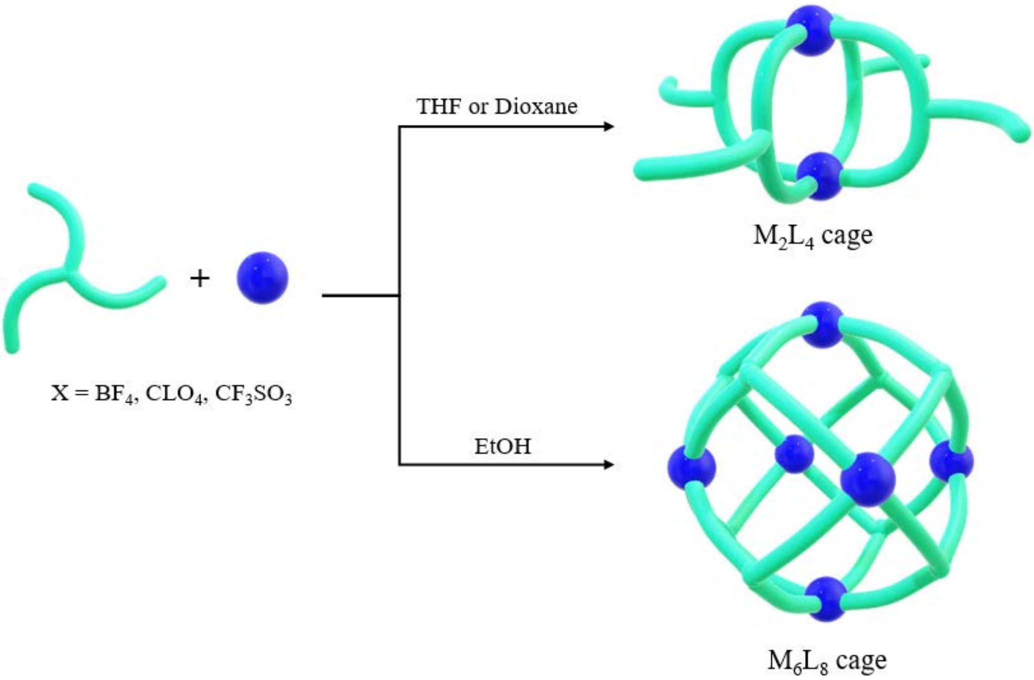
Poster Presentation : **INOR.P-33**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Solvent-Dependent Self-Assembly of CuX_2 with a C_3-Symmetric Tridentate Ligand: Formation of Stable M_2L_4 and M_6L_8 Cages

Kim Daeun, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

Self-assembly of CuX_2 (X = BF_4, ClO_4, CF_3SO_3) with new C_3-symmetric tridentate $5,5^{'},5^{''}$-(((2,4,6-trimethylbenzene-1,3,5-triyl)tris(methylene))tris(oxy))triisoquinoline (L) gives rise to single crystals of stable M_2L_4, M_6L_8 cages depending on the solvent. Notably, within M_2L_4 cages, one site of the three-dentate ligand remains uncoordinated, extending outside the cage. Conversely, in the cage formed by the trifluorosulfate anion, the uncoordinated site of the ligand is inwardly folded into the cage structure.


THF or Dioxane
M_2L_4 cage
+
X = BF_4, CLO_4, CF_3SO_3
EtOH
M_6L_8 cage

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Poster Presentation : **INOR.P-34**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

The Synthesis of Colloidal Silicon-Based Hollow Nanostructures through Solid State Reaction and their Bio-Application

Jeonghun Choi, In Su Lee*

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

Despite tremendous application potential, controlling the fragile Si nanostructures such as hollow-porous thin nanoshells under high-temperature solid-state reactions(SSR) is a synthetic challenge. In the present work, we introduce a SSR-guiding stratum, an embedded nanospace containing catalytic metal-silicide at a predetermined radial distance inside silica nanosphere to guide and confine the preferable growth of Si product-layer well-segregated from the rest of the volume as a result of stratum-directed phase separation process. This strategy synthesized M/Silicon (Si)-based hollow porous nanostructures (M/Si-HPNSs, M = Pd, Pt etc.) from < 100 nm silica NPs with high structural preservation under high temperature MTR conditions. The pre-constructed M-silicide stratum decided the location of newly emerging Si phase while the evolving MgO phase acted as cast, protected the HPNS during high-temperature thermal conversion and resulted to the thin porous shell of M/Si-HPNS. Due to the well-protected self-confinement, M/Si-HPNSs were conveniently dispersed as colloidal solutions in bio-relevant media, exhibiting the characteristic photoluminescence, cargo loading, and photocatalytic properties and were easily internalized inside the living cells for biorthogonal catalysis applications.

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Poster Presentation : **INOR.P-35**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis, Characterization, and Reactivity of a Highly Oxidative Mononuclear Manganese(IV)–Bis(Fluoro) Complex

Yu jeong Lee, Jaeheung Cho[1,*]

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

Recently, transition-metal terminal nonoxo complexes have shown a remarkable ability to activate and functionalize C–H bonds via proton-coupled electron transfer (PCET). Here we report the first example of a mononuclear manganese(IV) bis(fluoro) complex bearing a tetradentate pyridinophane ligand, $[Mn^{IV}(TBDAP)(F)_2]^{2+}$ (3), with an X-ray single crystal structure and physicochemical characterization. The manganese(IV) bis(fluoro) complex has a very high reduction potential of 1.61 V vs SCE, thereby enabling the four-electron oxidation of mesitylene to 3,5-dimethylbenzaldehyde. Kinetic studies, including the kinetic isotope effect and employment of other toluene derivatives, reveal the electron transfer (ET)-driven PCET in the C–H bond activation of mesitylene by 3. This novel metal halide intermediate would be prominently valuable for expanding transition-metal halide chemistry.

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Poster Presentation : **INOR.P-36**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Influence of Solvents on Catalytic C−H Bond Oxidation by a Copper(II)−Alkylperoxo Complex

Yuri Lee, Jaeheung Cho[*]

Department of Chemistry, UNIST, Korea

Oxidation of unactivated alkanes, which requires substantial energy for conversion to valuable organic chemicals, is a major challenge in both industry and academia. Herein, we describe how solvents affect and improve the catalytic oxidation ability of a mononuclear copper(II)−alkylperoxo complex, $[Cu^{II}(^{i}Pr_3\text{-tren})(OOC(CH_3)_2Ph)]^+$ (1, $^{i}Pr_3$-tren = tris[2-(isopropylamino)ethyl]amine), toward hydrocarbon substrates. 1 was prepared by adding cumene hydroperoxide and triethylamine to the solution of $[Cu(^{i}Pr_3\text{-tren})(CH_3CN)]^{2+}$, which was characterized using various physicochemical methods. Product analyses, along with theoretical calculations, indicate that homolytic O−O bond cleavage occurs during the thermal decomposition of 1 at 60 °C in various solvents such as CH_3CN, CH_3COCH_3, $C_6H_5CF_3$, and C_6H_6. Both experiment results and density functional theory (DFT) calculations supported variations in the catalytic activity of 1 depending on solvents. In CH_3CN and CH_3COCH_3, 1 activates weak C−H bonds (bond dissociation energy (BDE) ≤ ~ 81.6 kcal mol−1), while 1 in $C_6H_5CF_3$ and C_6H_6 can oxidize slightly stronger C−H bonds with a BDE of up to 84.5 kcal mol^{-1}. In supercritical carbon dioxide (SC-CO_2), 1 can oxidize alkanes with strong C−H bonds, such as cyclohexane (99.5 kcal mol^{-1}). The enhanced C−H bond oxidation of 1 in $C_6H_5CF_3$, C_6H_6, and SC-CO_2 was generally attributed to two different factors: (a) the nonpolarity of the solvent and (b) the absence of $C(sp^3)$−H bonds in the solvent. Interestingly, in CH_2Cl_2, a nonpolar solvent with C(sp3)−H bonds, 1 exhibited similar reactivity to that in $C_6H_5CF_3$, indicating that nonpolar solvents enhance the catalytic ability of copper(II)−cumylperoxo complexes to abstract hydrogen atoms from substrates, regardless of the presence of $C(sp^3)$−H bonds in solvent molecules. DFT calculations employing an implicit solvent model further supported the enhanced reactivity, without the need to account for the presence of $C(sp^3)$−H bond. The reactivity of the different possible reactive

intermediates arising from the catalytic oxidation was also explored using DFT calculations. This study provides a perspective on how solvents can be utilized to modulate catalytic effects on C−H bond activation.

Poster Presentation : **INOR.P-37**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Syntheses, Structures, and Optical Properties of Chiral Hybrid Metal Halides

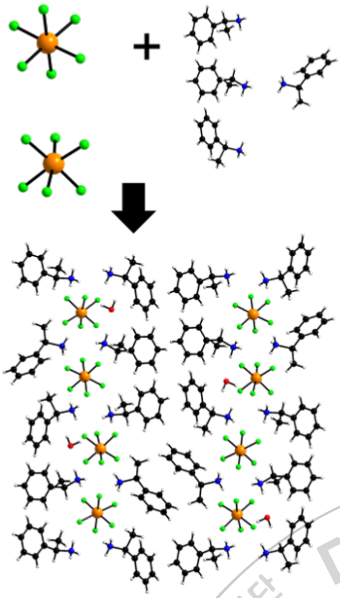
Kyungmo Kim, **Kang Min Ok**[1,*]

department of chemistry, Sogang University, Korea

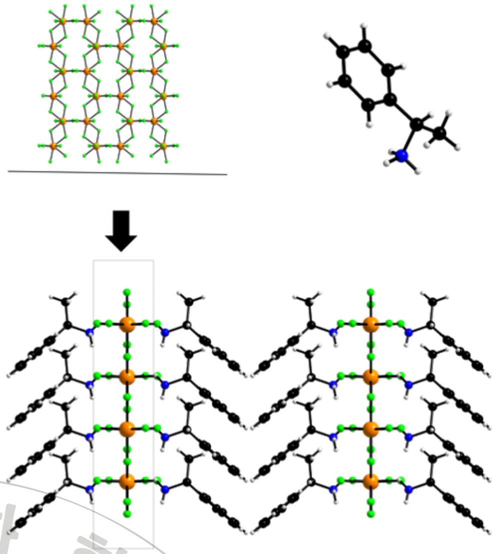
[1]*Department of Chemistry, Sogang University, Korea*

Hybrid organic-inorganic metal halides (HOMHs) have attracted significant attention due to their non-centrosymmetric (NCS) structures, which result in interesting properties such as second harmonic generation (SHG) and ferroelectricity, etc. Since the chiral space group belongs to one of the NCS crystal classes, introducing chirality by utilizing chiral organic ligands in HOMHs is a promising approach for systematically synthesizing novel NCS HOMH materials. For the type of metal in chiral HOMHs, hafnium (Hf), as a d^0 transition metal (TM) with the lowest electronegativity, has garnered significant interest for the following reasons: Firstly, the weak electronegativity of TMs, coupled with the strong electronegativity of fluorine, collectively enhances the ionic nature of the target materials, resulting in an enlarged band gap. Secondly, the Hf cation exhibits a wide range of coordination modes, making it a favorable metal for various polyhedral structures.In this work, we have successfully synthesized two different types of Hf-based HOMHs, namely two-dimensional (2D) (R/S)-1 and zero-dimensional (0D) (R/S)-2, via slow evaporation methods. Single crystal X-ray diffraction indicates that these two types of the title compounds crystallize in the NCS polar space group $C2$ and the nonpolar space group $P2_12_12_1$, respectively. This chiral-polar 2D (R/S)-1 reveals SHG efficiencies of approximately 0.4 times that of KH_2PO_4, while chiral-nonpolar 0D (R/S)-2 exhibits approximately 0.2 times that of KH_2PO_4. This poster presentation will cover detailed syntheses, crystal structures, and optical properties.

➢ **0D Structure**



➢ **2D Structure**



Poster Presentation : **INOR.P-38**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

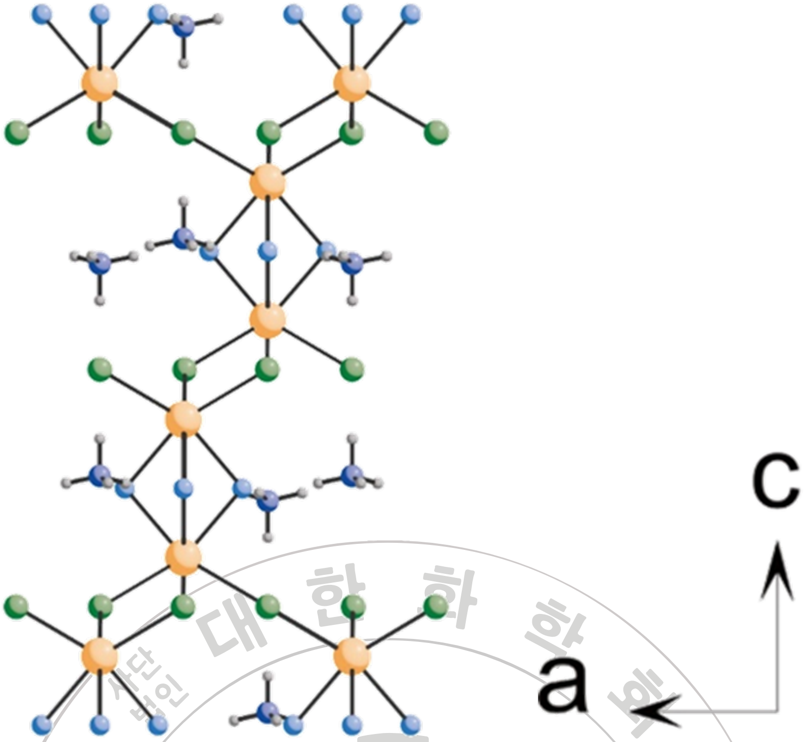
Synthesis, structure, and characterizations of non-centrosymmetric cadmium mixed halides

<u>Seunghun Choi</u>, Kang Min Ok[1,*]

department of chemistry, Sogang University, Korea

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

Single crystals of two cadmium mixed halides have been successfully synthesized using the hydrothermal method. Single crystal X-ray diffraction analysis reveals that both compounds crystallize in the noncentrosymmetric trigonal space group, *R*32, sharing isostructural 3D arrangements. Each compound features cadmium cations bonded to three fluorides and three halides (Cl^- for compound 1 and Br^- for compound 2), resulting in significant distortion along the C_3 axis. UV-vis diffuse reflectance spectra indicate large band gaps of 5.80 and 4.74 eV, respectively, attributed to the highly electronegative halides. Notably, powder second-harmonic generation (SHG) measurements of compound 1 and 2, using 1064 nm radiation, demonstrate strong SHG efficiency of, 2.0 and 6.6 times that of KH_2PO_4, respectively. Additionally, comprehensive characterization through powder X-ray diffraction, thermogravimetric analysis, and density functional theory calculations further elucidates the structural and optical properties of the title compounds. Detailed findings are presented in this poster presentation.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a

Poster Presentation : **INOR.P-39**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Structural and electrochemical characterization of 5,5-disubstituted-5H-dibenzo[b,d]silole

Min-Kyoung Kim, Young Tae Park[1,*]

Keimyung University, Korea

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

2,2-Dibromobiphenyl was prepared by dimerization of 1,2-dibromobenzene using *n*-butyllithium at -78℃ utilizing dry ice bath in THF solvent. 5,5-Disubstituted-5H-dibenzo[b,d]silole (R = Et, *n*-Hex, Phenyl) were produced through reactions of the prepared 2,2-dibrombiphenyl with *n*-butyllithium and dichlorodisubstitutedsilane (R = Et, *n*-Hex, Phenyl) in THF solvent, respectively. After the reaction was completed, the lithium salts were removed by washing with a dilute HCl aqueous solution. The crude products were extracted with ether and distilled water, and further purified by recrystallization in ethanol. The obtained products were soluble in usual organic solvents such as tetrahydrofuran and dichloromethane. All the prepared materials were characterized by ^{1}H, ^{13}C, ^{29}Si NMR, IR, TGA and UV-Vis spectroscopic methods. The electrochemical properties of the 5,5-diphenyl-5H-benzo[b,d]silole as anode materials for lithium-ion batteries, for example, C-rate performance and long cycling performance, were examined, particularly.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).

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Poster Presentation : **INOR.P-40**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Kinetic study of organic reactions by optical microscopy

Daeha Seo*, Minsoo Park

Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea

Mechanistic investigations are essential for understanding the insights and improving the efficiency of organic reactions. These studies involve traditional experiments, such as a synthesis of reaction intermediates, isotope labeling, kinetic isotope effect, Hammet plot, etc. Data that is typically concealed by methods averaging across groups can be revealed through experiments on single entities. We introduce a dependable approach using total internal reflection fluorescence microscopy, which utilizes organic dyes to observe the chemical behavior of singular molecules in real-time.. Due to fluctuations in the conjugation bond length and quantum yield, we may be able to observe the reaction process at the single-molecule level using TIRF. This method illustrates the optical properties of each intermediate or transition state, which are typically difficult to observe in time trajectories.

Kinetic study of organic reactions by optical microscopy

Minsoo Park[1], Wonhee Lee[1], Sunggi Lee[1,*], Daeha Seo[1,*]

[1]Department of Physics and Chemistry, DGIST, Daegu, 42988, South Korea

Mechanistic investigations are essential for understanding the insights and improving the efficiency of organic reactions. These studies involve traditional experiments, such as a synthesis of reaction intermediates, isotope labeling, kinetic isotope effect, Hammet plot, etc. Data that is typically concealed by methods averaging across groups can be revealed through experiments on single entities. We introduce a dependable approach using total internal reflection fluorescence microscopy, which utilizes organic dyes to observe the chemical behavior of singular molecules in real-time.. Due to fluctuations in the conjugation bond length and quantum yield, we may be able to observe the reaction process at the single-molecule level using TIRF. This method illustrates the optical properties of each intermediate or transition state, which are typically difficult to observe in time trajectories.

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Poster Presentation : **INOR.P-41**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Surface Chemistry of Extracellular Vesicles through Modular Approach

JuHee Jang

Emerging material science, Daegu Gyeongbuk Institute of Science & Technology, Korea

Extracellular vesicles (EVs), lipid bilayer structures of 50-200 nm containing proteins, growth factors, and nucleic acids, hold potential for clinical use in therapy and drug delivery. However, their low specificity necessitates surface engineering to improve target delivery and therapeutic efficacy. Current methods for EV surface engineering are categorized into genetic manipulation and chemical techniques, each presenting its own set of limitations. Genetic manipulation requires repetitive cellular engineering, which is time-consuming and can decrease engineering efficiency, with the range of engineerable molecules being limited to proteins. Conversely, chemical methods are constrained by the stability of engineered molecules, which may not remain stable over long periods or in specific environments.This study introduces a SNAP-tag mediated EV surface engineering technique, utilizing the Benzyl Guanine linker (BG linker) to facilitate the formation of stable covalent bonds. The BG linker specifically forms covalent bonds with the SNAP-tag, enabling stable surface engineering. This approach simplifies the surface engineering process and endows EVs with the modularity to efficiently bind a wide range of molecules. The reaction between the SNAP-tag and BG-linker is highly specific, without cross-reactivity, and it has been confirmed that the SNAP-tag exists as monomers on the plasma membrane without interacting with other molecules. This minimizes the impact on other surface molecules of EVs and reduces the potential for functional alteration of EVs during the engineering process.

Poster Presentation : **INOR.P-42**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Strong coordination at open-metal sites enhances hydrolytic stability of metal-organic frameworks.

JaeHyeuk Choi, Nak Cheon Jeong[1,*]

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Metal-organic frameworks (MOFs) possessing open metal sites (OMS) can be utilized as catalysts. However, a drawback of OMS-containing MOFs is their low hydrolytic stability. Consequently, various methods such as metal node reduction, polymer coating, and the use of hydrophobic ligands have been employed to enhance the stability of MOFs toward moisture.Nevertheless, research on the increase in hydrolytic stability due to the coordination of guest molecules within MOFs has been scarce, and studies on the varying degrees of protection afforded by molecules of varying coordination strength have not been conducted.Therefore, in our study, we investigated the increase in hydrolytic stability according to the coordination strength of various molecules bound to HKUST-1. Our results showed that DMSO, DMF and EtOH enhance the stability of HKUST-1 towards water. PXRD measurements showed that DMSO-coordinated HKUST-1 is the most stable material compared to DMF- or EtOH-coordinated HKUST-1. Nonetheless, HKUST-1 with OMS displayed the lowest hydrolytic stability. These results confirm that strongly coordinated molecules to metal centers can improve the hydrolytic stability of MOFs with OMS.

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Poster Presentation : **INOR.P-43**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Solvent-Triggered Photo-Reactivity of One-Dimensional Coordination Polymers

TaeHun Kim, Kyunghye Ju, In-Hyeok Park*

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

The incorporation of di-olefin ligands with suitable spacing within metal-organic frameworks/Coordination Polymers (CPs) structures becomes crucial for facilitating efficient photochemical reactions. The controlled alignment and proximity of these olefinic groups within the MOF framework play a pivotal role in dictating the photo-reactivity of the material. Schmidt's criteria provide valuable insights into the optimal distance between olefins for promoting photochemical transformations, typically falling within the range of 3.6-4.1 Å. In this study, we focus on the synthesis and characterization of photo-reactive MOFs utilizing di-olefinic ligands, specifically bpeb (di-olefin ligand) and its derivatives, within the framework. Firstly, a 1D railroad MOF $[Zn_2(bpeb)_2(adc)_4]$ (**1**) is synthesized, followed by the synthesis of a structurally similar MOF $[Zn_2(bpeb)_2(adc)_3(fa)]$ (**2**), where formate (fa) groups are introduced through partial pyrolysis of DMF. Notably, the incorporation of formate groups offers an additional avenue for modulating the photo-reactivity of the MOF framework. Subsequently, the photo-dimerized MOF $[Zn_2(bpbpvpcb)(adc)_3(fa)]$ (**3**) is synthesized via UV irradiation, wherein bpbpvpcb (1,2-bis(4-pyridyl)-3,4-bis[4-{2-(4-pyridyl)vinyl}phenyl]cyclobutane) serves as the dimer of bpeb. The parallel alignment of double bonds within the bpeb ligands in MOF (**2**) at a distance of 3.813 Å, as confirmed by structural analyses, satisfies Schmidt's criteria for photo-reactivity. Furthermore, the formation of cyclobutane rings in MOF (**3**) is corroborated through comprehensive spectroscopic techniques, including ^1H nuclear magnetic resonance and single-crystal X-ray crystallography. This work not only underscores the significance of controlled ligand spacing in governing photo-reactivity within MOF frameworks but also demonstrates the utility of photochemical transformations in engineering novel functionalities in these versatile materials.

Poster Presentation : **INOR.P-44**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Solution-Processible 2D Conducting Metal-Organic Framework with Proton-Dopable Charge Transport

Geunchan Park, Monique C. Demuth[1], Christopher H. Hendon[1,*], Sarah Sunah Park[*]

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Electrically conductive 2D metal-organic frameworks (MOFs) have become crucial in various applications, including chemiresistive sensors, electrochemical catalysts, field-effect transistors, and energy storage devices. These applications were previously inaccessible due to challenges in carrier mobility and low electrical conductivity in MOFs. However, industrial implementation faces persistent obstacles, with limited synthetic control over their electrical or chemical properties, and typical synthesis yielding bulk powder with minimal processibility. To overcome these challenges, we employed a straightforward solvothermal method to synthesize crystalline 2D MOF bulk powder, introducing pendant amines with Brønsted-basic and π-electron-donating roles into the ligand. Our study explores the electronic structural effects of pendant amines through X-ray absorption spectroscopy, electrical property experiments, and DFT calculations, confirming it as a p-type conductor with enhanced electrical conductivity. Furthermore, within the framework structure, we observed the Brønsted-acidic and basic behavior of pendant amines without structural collapse through X-ray absorption spectroscopy. This behavior enables the liquefaction of bulk powder and the facile fabrication of large-area thin-film devices via a simple spin-coating process using the solution. This study signifies the synthesis of a novel 2D MOF with an aromatic tritopic ligand, showcasing its solution processibility. The ligand's ease of synthesis enhances its potential for diverse applications, inspiring researchers to explore its uses and investigate the synthesis of new 2D MOFs with unique characteristics.

Poster Presentation : **INOR.P-45**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Luminescence Properties in Atomically Defined Au_{25} Cluster-Based Superlattice

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

[1]*Beam Operation Team, Pohang Accelerator Laboratory, Korea*

Metal nanoclusters with isolated electronic structures have been the subject of research due to their intriguing optical properties, leading to active research on photoluminescence (PL) properties. Despite numerous studies on PL properties in the past two decades, fundamental questions regarding the mechanisms underlying PL remain unanswered. This challenge stems from the complex electron dynamics within nanoclusters and the difficulty in characterizing their structures precisely, hindering accurate structure-based interpretations. Therefore, there is a need for a method to analyze structure-based PL properties accurately.In our study, we present a straightforward approach for synthesizing single-crystal nanocluster-based superlattices that can be examined at the atomic level. We have successfully synthesized two distinct single-crystal nanocluster-based superlattices, which exhibit contrasting optical behaviors owing to different interactions and packing structures elucidated through single-crystal X-ray diffraction. This work will significantly advances the research field by providing comprehensive insights into the photophysical properties based on steady-state and time-resolved PL, along with electronic structure analysis using DFT calculations, shedding light on the diverse optical properties influenced by the structure.

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Poster Presentation : **INOR.P-46**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Etching-Free Synthesis of Silicon@Graphite Yolk-Shell Structure for High-Efficiency Lithium-ion Battery Anode

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With the technical growth of electronics and electric vehicles, the development of stable, high-capacity lithium-ion batteries is a reality to come true. Therefore, Silicon, which is known as having the highest capacity among the anode materials of lithium-ion batteries, is one of the biggest issues. However, the volume of silicon expands about 4 times during the charge-discharge process, which is the main problem of the silicon anode. In addition, in the first cycle, silicon reacts excessively with the electrolyte to generate a solid-interface layer (SEI layer) due to volume expansion, which reduces the coulombic efficiency, resulting in a lower battery capacity.Herein, we synthesize the Si@G yolk-shell structure via surface polymer coating and chemical vapor deposition method based on micron-sized silicon. Micron-sized silicon was functionalized using 3-(Trimethoxysilyl)propyl methacrylate (MPS) and subsequently coated with a polymethylmethacrylate (PMMA), a polymer that decomposes upon heating, followed by a polydopamine a polymer capable of carbonization. This process led to create a yolk-shell silicon-carbon composite structure that does not require any additional etching steps due to the thermal decomposition of PMMA during the carbonization process. Further enhancement was achieved by controlling the surface area through CVD using acetonitrile, which effectively suppressed the formation of SEI layers on the carbon surface. This strategic approach yielded Si@G with high initial efficiency and significantly improved capacity and longevity performances for lithium-ion battery anode.

Poster Presentation : **INOR.P-47**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Dinitrogen Activation with a Molybdenum Complex

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The Haber-Bosch process (HBP) is one of the most important chemical processes, which has been extensively utilized in the industrial ammonia production. Although it provides a major nitrogen source for the production of fertilizer and various synthetic N-containing chemical products, the HBP is confronted with significant energy or environment problems. Consequently, there have been numerous efforts to develop an alternative process by utilizing molecular catalysts, which can be operated under milder homogeneous catalytic conditions. One of the main challenges is to deal with the cleavage of a N–N triple bond exhibiting a considerably high activation barrier and its complete cleavage into a metal nitride species to produce ammonia. Herein, we present the formation of the molybdenum nitrido complex exhibiting the unique dinuclear structure resulting from the activation of atmospheric N_2. A diazenido dimolybdenum complex was synthesized from 2-electron reduction of a trichloro molybdenum complex under N_2 atmosphere and its further reduction generates the molybdenum(V) nitride species. Both thermally stable molybdenum species were fully characterized by various spectroscopic tools. Notably, the solid-state structure of the molybdenum(V) nitrido complex shows unprecedented dinuclear dinitride, which contains a weakly activated dinitrogen ligand. Moreover, the crucial structural difference of the PNP pincer platforms between two N_2-bridged complexes is also quite interesting, arising from orbital mixing which necessitates further studies. The impressive feature of the system can provide the platform for introduction of a nitrogen atom into π-acidic ligands such as C–N bond formation beyond ammonia production in the mild conditions.

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Poster Presentation : **INOR.P-48**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Early Onset Diagnosis in CVDs Patients via Homocysteine Specific Redox Active Fluorogenic Probe in Blood Plasma

Snehasish Debnath, Jusung An, Jungryun Kim, Hyeonji Rha, Jaewon Kim, Eunji Kim, Huiyeon Moon, Ki-ppeum Lee[1], Yubin Lee[1], Jong Seung Kim[*]

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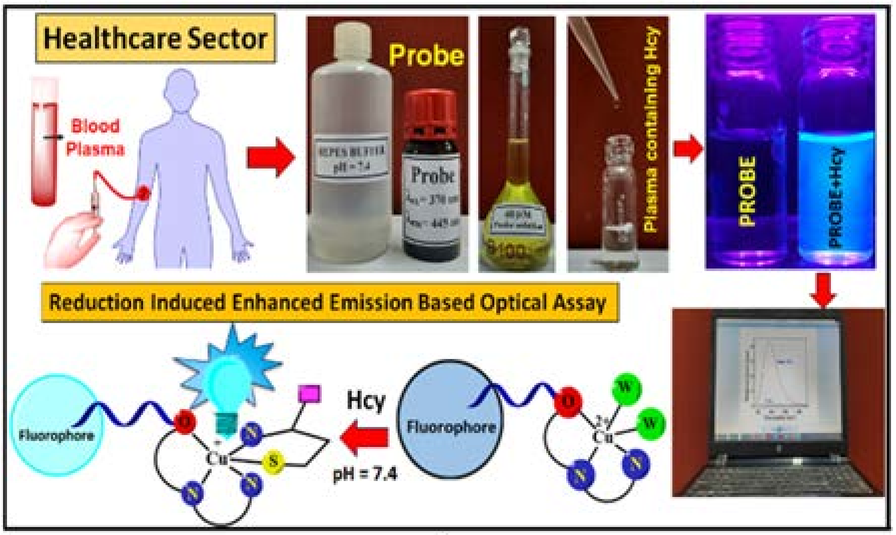
[1]Korea University, Korea

Cardiovascular diseases (CVDs) have threatened human lives for decades, accounting for approximately 17.9 million lives each year.1 In recent times, the association of elevated homocysteine (Hcy) levels with cardiovascular diseases (CVDs) has provoked an immense interest in the primitive stage identification of CVDs.2 Mounting evidence suggest that the highly reactive sulfhydryl group of Hcy is accountable for platelet aggregation and oxidative stress, leading to CVDs.2 Thus, health initiatives worldwide demand affordable point-of-care (POC) Hcy specific diagnostic tools offering the right treatment at the right time for effective CVD therapeutic control. Despite recent progress in fighting with these fatal diseases, the best approach for achieving an early stage cost-effective diagnosis that will be operative in low-resource settings remained unsuccessful. In view of this, a major drive for developing point-of-care (POC) assay for measuring plasma Hcy could facilitate early detection of CVD as well as individualized therapy monitoring. Normal level of Hcy ranges between 5-15 μM, Hcy levels $\geq$ 15 μM, $\geq$ 30 μM and $\geq$ 100 μM indicates moderate, intermediate and severe conditions of hyperhomocysteinemia (HHcy), respectively.2 Herein, a series of water soluble redox active iminocoumarin-ensembled Cu complexes has been developed, which displays ‘off-to-on’ response towards Hcy.2 EPR and UV-vis studies has established reduction-induced-emission-enhancement of the sensor for its ‘off-to-on’ behavior with Hcy. Furthermore, we demonstrate clinical testing of our probe in human plasma of cardiac patients and healthy volunteers. Validation using traditional HPLC and reliability against clinically approved commercial immunoassay kit confirms the diagnostic potential of the optical sensor. The presented optical sensor demonstrates the feasibility for the development of Hcy-selective diagnostic kit to be suitable for point-of-care uses. References1. Angew Chem. Int. Ed., 2023, 135, e202310408.2. Chem Commun., 2022,58, 9210-9213.



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Poster Presentation : **INOR.P-49**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of nanofractals via cation exchange reactions for highly efficient electrocatalysts

Yujin Lee, Jongsik Park[*]

Department of Chemistry, Kyonggi University, Korea

Electrocatalysts hold great promise for energy conversion and storage, so the performance of electrocatalysts plays an important role in energy conversion and storage technologies.In general, strategies to increase the surface area of nanocatalysts with possessing numerous active sites have been investigated to ensure high catalytic activity in electrocatalysts.However, the synthetic methodology for the bulk formation of active sites within nanoparticles is very challenging due to the high surface energy resulting from the unsaturated coordination state.Herein, we performed the co-decomposition of transition metal precursor and CuSCN, leading to regiospecific exchange of transition metals at the active sites of copper sulfide templates.Based on the corner-protected copper sulfide templates, the remaining CuSCN precursor was thermally decomposed to the edges of $Cu_{2-x}S$, resulting in the formation of nanofractals with numerous active sites.This synthesis methodology can be utilized as highly efficient and cost-effective templates to replace previously reported noble metal-based electrochemical catalysts.

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Poster Presentation : **INOR.P-50**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Medium and high-entropy noble metal nanoparticles via sequential cation exchange

Ryunhyun Kim, Jongsik Park*

Department of Chemistry, Kyonggi University, Korea

Among the random mixtures of various components, medium and high-entropy alloy nanoparticles are being studied in fields such as catalyst design for the reason that their unique mixing state can tune their activity and enhance their stability. Previously reported methodologies for the synthesis of medium and high-entropy alloys suffer from several challenges, such as reduced surface area due to grain growth at high temperatures, which leads to decreased catalytic efficiency and difficult morphology control. To solve this problem, we used a cation exchange method, which is carried out at relatively low temperatures, to distribute the various components in large numbers within the crystal structure. $Cu_{1.81}S$ was chosen as the host template for the cation exchange process, and by sequentially exchange of two noble metal cations, we succeeded in synthesising nanoparticles with novel medium and high-entropy alloy compositions that have not been reported previously. This strategy for synthesising medium and high-entropy alloy nanoparticles using cation exchange methods is expected to allow tuning of the morphology and composition ratios between compositions, and is expected to lead to catalysts with unique physicochemical properties using novel compositions not previously reported.

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Poster Presentation : **INOR.P-51**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Heterointerfaces Engineering of $CuS/Ag_2S/CuS$ nanosandwich *via* post-synthetic modification

Suin Jo, **Jongsik Park**[1,*]

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

Hetero-nanoparticles have been largely investigated for the highly efficient photo- and electrocatalysts due to the unprecedented physicochemical properties induced by each juxtaposed domain. Typically, the successful formation of heterointerfaces within nanoparticles has been determined when the degree of lattice mismatch between the template and the newly formed material is minimized. From this point of view, it is challenging to synthesize thermodynamically unfavorable types of heterointerfaces. Herein, we show that the phase transition at the specific material phase could evolve the surface strain at the already formed heterointerface, resulting in atomic migration to minimize the overall surface energy. As a result, we synthesized $CuS/Ag_2S/CuS$ nanosandwich, which has not been previously reported through the covellite-based cation exchange reactions. Through this method, we anticipate not only expanding the complex nanostructural libraries but also foresee significant effects on the catalytic activity in various fields due to variations in the heterointerface area, which can influence the efficiency of hole-electron transfer within the particles.

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Poster Presentation : **INOR.P-52**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Secondary Sphere Impact on Organometallic Catalysts in Photochemical CO2 Reduction:Tailoring Product Selectivity through Alcohol and Alkyloxy Tethering Ligands

Min-Jong Bong, Daehan Lee, Seong Woon Jeong, Myung Jae Lee, Ho-Jin Son[1,*]

Department of Advanced Materials Chemistry, Korea University, Korea

[1]*Department of Advanced Materials Chemistry, Korea University, Sejong, Korea*

Secondary coordination effects represent a promising and effective strategy to enhance the catalytic performance and product selectivity in organic-metallic catalysis for CO_2 reduction. Addressing the drawbacks of (bpy)Mn(I)CO_3Br photocatalyst, characterized by (bpy)$(CO)_3$Mn-Mn$(CO)_3$(bpy) dimerization and subsequent reduced selectivity, we propose a novel (R-bpy)Mn(I)CO3Br complex incorporating functional groups (-OH, OCH_3, or OCH_2CH_3) attached to the ortho position of the 2,2'-bipyridine (bpy) ligand. Photolysis experiments demonstrate that the catalyst with the newly introduced form of bipyridine ligand exhibits enhanced efficiency in CO_2-to-formate conversion compared to the nontethered case, accompanied by a notable increase in product selectivity. FTIR analyses reveal that the catalyst with the additional tethering group effectively controls Mn-Mn dimerization, facilitating rapid proton supply and inducing the transformation to [(R-bpy)Mn(η^1-OCHO)$(CO)_3$]. Simultaneously, stabilization of Mn-formate intermediates through hydrogen bonding with the pendant group promotes smooth conversion to formate. Furthermore, increasing the number of pendant tethering groups leads to even higher efficiency in CO_2-to-formate conversion (TON >290) and product selectivity exceeding 90%. These findings underscore the effectiveness of the proposed strategy in mitigating dimerization-related drawbacks and improving the overall performance of CO_2 reduction catalysts.

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Poster Presentation : **INOR.P-53**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Solvated electrons from alkali metals at room temperature

Changmin Choi, Jongcheol Seo[1,*], Hee Cheul Choi[1,*]

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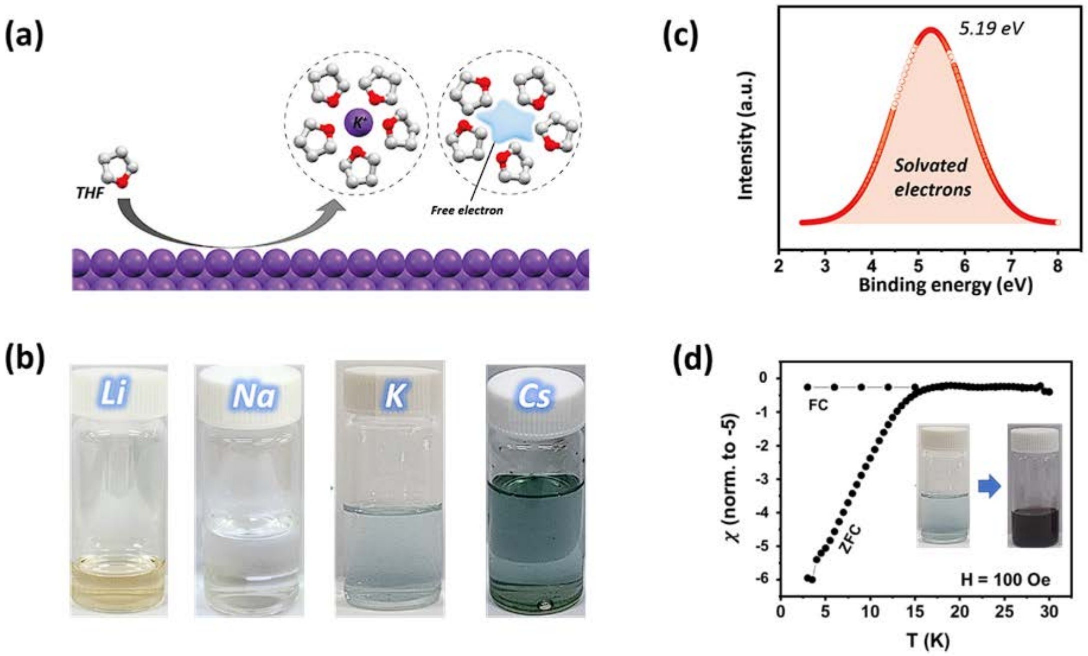
[1]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Solvated electrons are of great interest not only for fundamental research including electronic dynamics, but also for various potential applications such as energy sources in batteries and high energy catalysis. This presentation introduces a novel method for generating solvated electrons from alkali metals in tetrahydrofuran (THF) at room temperature, enhancing their accessibility and practicality. Employing a graphene liquid cell for photoelectron spectroscopy, we investigated the binding energies between these solvated electrons and the solvent, gaining valuable insights into their interactions.A notable achievement of our research is the prolonged stability of solvated electrons in an argon atmosphere for over seven days. This breakthrough, coupled with the simplicity of our synthesis process, underscores the feasibility of our method for diverse applications. We successfully identified AM(THF)n+ complexes, essential for stabilizing solvated electrons.The practical implications of our findings are significant. We demonstrated the application of this technique in doping C60 fullerene, leading to the synthesis of superconductors. Furthermore, our method proved effective in powering LED bulbs, showcasing its potential in electric energy systems.This research goes beyond presenting a new technique for solvated electron generation. It provides a deeper understanding of their behavior, paving the way for novel applications in energy storage, chemical reactions, and electronic device manufacturing, leveraging the unique properties of solvated electrons.


(a)
THF
K⁺
Free electron
(c)
Intensity (a.u.)
5.19 eV
Solvated electrons
Binding energy (eV)
2
3
4
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7
8
(b)
Li
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Poster Presentation : **INOR.P-54**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Exploring Reactivity Control in a Novel Cobalt-Oxo Complex: Leveraging the Outer Coordination Sphere Effect Beyond Primary and Secondary Coordination

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[1] *Department of Chemistry & Nanoscience, Ewha Womans University, Korea*

The outer coordination sphere effect impacts the environment surrounding a metalloenzyme's active site, thereby influencing its catalytic properties. It plays a crucial role in various energy conversion reactions and the catalytic activity of metal ions within the active site, affecting processes like electron and proton transfer, as well as substrate binding. Nature's enzymes use manganese and iron-containing metallocofactors to catalyze reactions involving oxygen atoms, such as alkane hydroxylation and olefin epoxidation. Metal-oxo complexes are proposed intermediates, facilitating key steps like C–H bond activation and oxygen atom transfer. In contrast to the manganese and iron congeners, cobalt-oxo complexes are absent in biological systems. This rarity is attributed to the structural instability of metal-oxygen double bonds in Group 9-11 metals beyond iron, known as the "oxo wall," historically impeding cobalt's involvement in oxidation reactions. Herein, we report how the outer coordination sphere affects reactivity in a new cobalt-oxo complex. In addition to examining the primary and secondary coordination effects, we investigated the effect of redox-inactive cation in modulating the complex reactivity by its outer coordination sphere effect.

Poster Presentation : **INOR.P-55**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Enhanced CO_2 Reduction to CO Utilizing TiO_2-Adsorbed Cationic Ir(III) Complexes with pendant moieties:In a TiO_2/ReP Hybrid Catalyst System

<u>Seung Hwan Cha</u>, Seong Woon Jeong, Min-Jong Bong, Myung Jae Lee, Ho-Jin Son[1,*]

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[1]*Department of Advanced Materials Chemistry, Korea University, Sejong, Korea*

A series of cationic Ir(III) complexes ($[Ir(piq)_2(bpy\text{-}X_2)]^+$ ($Ir\text{-}X^+$: piq = (1-phenylisoquinoline; bpy-X_2 = 4,4´-X_2-2,2´-bipyridine (X = pyridyl, methyl pyridyl, phenyl, none)) were utilized as visible-light photosensitizers for the CO_2 reduction to CO using a hybrid catalyst (TiO_2/ReP). The hybrid catalyst was prepared by anchoring Re(4,4´-Y_2-bpy)$(CO)_3$Cl (ReP; Y = $CH_2PO(OH)_2$) on TiO_2 particles. Irradiation of a solution containing $Ir\text{-}X^+$, TiO_2/ReP particles, and an electron donor (1,3-dimethyl-2-phenyl-1,3-dihydrobenzimidazole) in N,N-dimethylformamide with 3 vol% H_2O at wavelengths greater than 500 nm resulted in efficient CO_2 reduction to CO. The efficiencies followed the order X = methyl pyridyl > pyridyl > phenyl > none. The synthesized Ir(III) photosensitizers with pendant pyridyl moieties, facilitating adsorption onto TiO_2, exhibited significantly enhanced CO_2-to-CO conversion activities compared to control photosensitizers lacking adsorbing moieties.

Poster Presentation : **INOR.P-56**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Ionothermal synthesis of early transition metal 2D Metal-organic frameworks

<u>Hyeonwoo Lee</u>, Hee Cheul Choi[*]

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

The early transition Metal-organic frameworks (ETMOFs) are potential high conductive systems for their varied oxidation states and redox capabilities. Unfortunately, attempts to make ETMOFs frequently end up with the formation of metal-oxo clusters that severely impede charge transfer within the MOFs, thereby diminishing their conductivity potential. To overcome this barrier, our study introduces ionothermal synthesis as a strategic approach to fabricate MOFs devoid of these obstructive metal-oxo clusters. Utilizing ETM precursors that can undergo ionothermal reactions can avoid the formation of metal-oxo clusters. In this presentation, I will introduce our recent success in the synthesis of Ti2(THQ)3 and Nb3(THQ)2 MOFs via ionothermal synthesis using titanium isopropoxide and niobium ethoxide precursors. Being conducted under inert conditions, this synthesis promotes the formation of MOFs with mononuclear secondary building units (SBUs) and a honeycomb structure, which are ideal for facilitating seamless charge transport.The notable electrical conductivity of Ti2(THQ)3 MOF, recorded at 1.2×10-5 S cm-1, underscores the success of ionothermal synthesis in circumventing the limitations previously imposed by metal-oxo clusters in ETM-based MOFs. This breakthrough not only paves the way for the development of MOFs with enhanced electrical properties but also broadens their potential applications, from electronics to catalysis. It sets a promising direction for future research focused on expanding the repertoire of conductive MOFs through ionothermal synthesis, suggesting a transformative impact on their industrial applications.

Poster Presentation : **INOR.P-57**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Fabrication of quasi-2D perovskite thin films via two-step deposition method

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

Quasi-2D halide perovskites are superior to the conventional 2D or 3D halide perovskites for their high heat and moisture stability while retaining their outstanding light absorption and charge transport property. However, it is extremely difficult to obtain pure quasi 2D perovskite thin films via conventional one-step coating method because of the colloidal characteristic of precursor solution. To avoid this issue, we developed a two-step method for the preparation of quasi-2D perovskite thin films. In this presentation, we introduce the two-step deposition method to obtain the Dion-Jacobson quasi-2D halide perovskite thin films with suppressed 3D perovskite phase. Especially, the effect of a stepwise introduction of two organic cations, 1,4-butyldiammonum (BDA) and methylammonium, making a huge influence on the suppression of the 3D perovskite phase will be discussed. An obvious absence of 3D perovskite phase was confirmed by UV-Vis spectroscopy and photoluminescence spectroscopy, and the importance of the structure and composition of intermediate films was systemically studied using X-ray diffraction and infrared spectroscopy. This study will open a new chapter of the preparation of perovskite thin films including phase-pure quasi-2D perovskites.

Poster Presentation : **INOR.P-58**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Computational elucidation of photo-induced reductive elimination mechanism of divalent organopalladium and organoplatinum complexes

<u>Minyoung Ju</u>, Jeongcheol Shin*

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Recent studies on the organonickel complexes have revealed that slow and rate-determining reductive elimination (RE) reactions of Ni(II) complexes can be accelerated by the photoexcitation, particularly through C-to-Ni CT excited states. Notably, RE reactions at the M(II) oxidation state are often rate-determining in various Pd-catalyzed cross-coupling reactions, and as well as kinetically inert Pt(II) complexes. Furthermore, Pd and Pt complexes are expected to exhibit photoreaction selectivity different from that of Ni analog, underscoring the importance of the mechanistic studies on the photo-induced RE reactions of Pd and Pt complexes. However, relatively fewer efforts were conducted to develop the photoreactions of Pd and Pt complexes, including photo-induced RE reactions. In this study, density functional theory (DFT) computations were employed to provide the mechanistic insights on the photo-induced RE reactions, in order to emphasize the accessibility of excited-state reactions of organometallic Pd and Pt complexes. Excited-state potential energy surfaces (PESs) were plotted onto the ground-state PESs to explore the excited-state behavior. Pd and Pt complexes with N,N,N’,N’-tetramethylethylenediamine (tmeda) and 1,10-phenanthroline (phen) ancillary ligands were employed to investigate the ground- and excited-state thermodynamics and kinetics of Me-Me, Me-Ph, and Ph-Ph bond-forming RE reactions (Figure 1a). M(phen)$(R)_2$ complexes have additional low-energy MLCT excited states compared to M(tmeda)$(R)_2$ complexes, implying better accessibility toward photoreactions (Figure 1b). This comparative study provides the insights onto the excited-state reactions of divalent organopalladium and organoplatinum complexes.

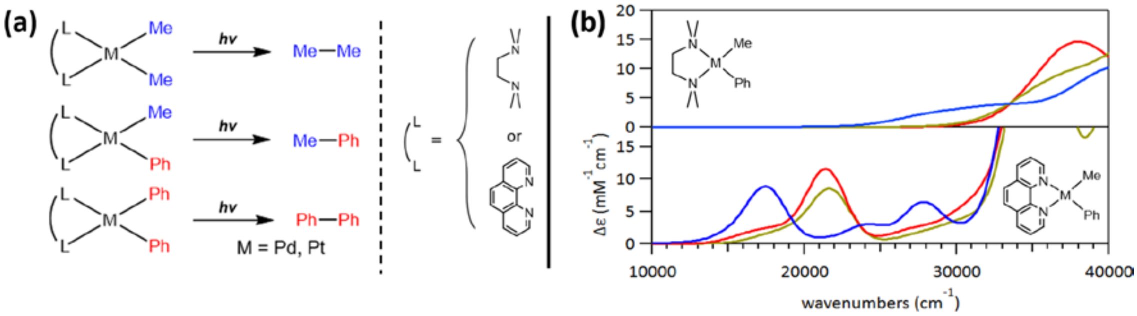

Figure 1. (a) Target photo-induced RE reactions and (b) DFT-simulated UV-Vis spectra of $M^{II}(L_2)(Me)(Ph)$ complexes, while L_2 = tmeda (top) and phen (bottom), M = Ni (**blue**), Pd (**yellow**), and Pt (**red**).

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Poster Presentation : **INOR.P-59**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Partially halogenated HKUST-1: tailoring the water adsorption properties of the Cu-based MOF through a mixed-linker strategy

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Water adsorbents must show a particular affinity towards water, but how strong this affinity is, will impact their performance on determined application and the temperature required for their regeneration. In this sense, metal-organic-frameworks (MOFs), porous hybrid crystalline materials conformed by metal clusters linked by organic moieties, can be easily designed to improve their hydrophilicity and to modulate their water adsorption kinetics. Nonetheless, low hydrolytic stability is a recurring drawback of MOFs, and it has impeded their widespread use as water adsorbents. Such is the case of HKUST-1, a copper(II)-based MOF with good water uptake and fast adsorption kinetics. An alternative to improve the hydrolytic stability of HKUST-1 is the introduction of certain functional groups, such as perfluorinated chains or ending -CF3 groups. However, this strategy has also reduced the total uptake capacity. Thus, customizing HKUST-1 for a given water-adsorption application requires a systematic control of the hydrophilicity without a significant loss of porosity. Although several studies have reported a mixed-linker approach to tailoring the adsorption properties of HKUST-1 for a wide range of probe molecules, the introduction of small amounts of halogen atoms (F, Cl, or Br) and its consequences on water adsorption properties of HKUST-1 has not been systematically addressed. In this work, we present a one-pot solvothermal synthesis of mixed-linker HKUST-1. The structural and textural properties of the obtained materials were evaluated, and the water adsorption performance was compared to pristine HKUST-1.

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Poster Presentation : **INOR.P-60**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Effect of growth temperature and pressure on the catalytic activity of MoS_2

Jeeung Kim, Joohyun Lim*

Department of Chemistry, Institute for Molecular Science and Fusion Technology, Multidimensional Genomics Research Center, Kangwon National University, Korea

MoS_2 is a non-precious metal catalyst for electrochemical hydrogen evolution reaction. Thanks to its abundant resources, it has garnered significant attention as an economically efficient catalyst. Previous studies have predominantly focused on modifying the properties of MoS_2 through elemental doping, phase transformations, vacancy formation, etc. Despite the catalytic activity of MoS_2 depending on various synthetic conditions, the relationship between them has not been systemically studied yet. We investigated the influence of reaction temperature and pressure on the catalytic activity of MoS_2. In this work, MoS_2 was synthesized on carbon cloth using a hydrothermal synthesis method. The synthesis involved temperature control and adjustment of the reaction volume for pressure control. Subsequently, the morphology, oxidation state, and crystalline phase of MoS_2 were analyzed using a scanning electron microscope, X-ray photoelectron spectroscopy, X-ray diffraction, and Raman spectroscopy. The catalytic activity as a hydrogen evolution reaction electrocatalyst was further confirmed through linear sweep voltammetry analysis. As the synthesis temperature and pressure increased, the morphology and crystalline phase of MoS_2 changed, with an increase in the Mo oxidation state. Optimal catalytic performance was observed under specific conditions. The detailed relationship between reaction conditions and catalytic performance will be discussed.

Poster Presentation : **INOR.P-61**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of New Mn(II) Structures by Flexible Ligand Design

HyunSeo Kim, Haeri Lee[1,*]

Department of chemistry, Hannam University, Korea
[1]*Department of Chemistry, Hannam University, Korea*

Recent studies have shown that metal complexes containing imidazole groups as electron donors can be rapidly formed and have a wide range of applications such as catalysts and containers for drug delivery systems. In our research group, we aim to create new metal complexes containing imidazole-donor ligands. New bis(monodentate) ligand was synthesized in two steps and characterized using FT-IR and 1H NMR analyses. Mn(II) coordination polymers were successfully formed as a crystalline solid from self-assembly of as-synthesized ligands and MnX2 (X = Cl, Br, I, NO3, ClO4). All crystal structures were analyzed by single-crystal X-ray diffractometer. Ongoing work is focused on further exploring the structural effects and consequences of Mn(II) coordination polymers. Through an in-depth study of these factors, we aim to improve our knowledge of the properties and potential applications of manganese-based coordination compounds.

Poster Presentation : **INOR.P-62**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Amplified Triplet Emission of Organic Periphery Groups by Exothermic Triplet−Triplet Energy Transfer from the ^{3}MLCT State of Pt(pmi)acac Core Complex to the ^{3}LC State of Geometrically Confined Carbazole/Naphthyl Tethers

Seong Woon Jeong, Seung Hwan Cha, Daehan Lee, Hyeongu Kang, Ho-Jin Son[1,*]

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[1]*Department of Advanced Materials Chemistry, Korea University, Sejong, Korea*

To investigate the excited-state properties of metal-organic bichromophores, including energy transfer mechanisms, a series of new heteroleptic N-heterocyclic carbene (NHC)-based platinum (Ⅱ) acetyl acetone (Pt(acac)) complexes were prepared by incorporating a peripheral naphthalene (Np) (Pt(Nppmi)acac : Pt(1-Nppmi)acac and Pt(2-Nppmi)acac) or carbazole (Cz) (Pt(Czpmi)acac : Pt(o-Czpmi)acac, Pt(m-Czpmi)acac, and Pt(p-Czpmi)acac) unit to the phenyl moiety of the phenylimidazole (pmi) ligand. Through a series of photophysical analyses and femtosecond time-resolved absorption (fs-TA) spectroscopy, it was discovered that the phosphorescence of the Pt core, (Pt(pmi)acac), was considerably quenched, while intense phosphorescence peaks arising from the excited triplet Np (^{3}Np*)/Cz (^{3}Cz*) species were primarily observed at room temperature (r.t.) and low temperature. Such amplified phosphorescence of the tethered organic Np and Cz units originated from triplet−triplet energy transfer (TTET) from the high-lying metal-to-ligand charge transfer (^{3}MLCT) state of the Pt(pmi)acac core to the ligand-centered triplet state (^{3}LC) of the peripheral Np and Cz units. This result indicates that the exothermic intramolecular energy transfer (IET) in the excited triplet state realizes the efficient phosphorescent emission of geometrically confined organic tethers.

Poster Presentation : **INOR.P-63**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Selective Formation of CO/Formate in the Photocatalytic CO_2 Reduction Catalysed by Half-Metallocene Ruthenium(II) Catalyst and Its Mechanistic Investigation

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Department of Advanced Materials Chemistry, Korea University, Korea

[1]*Department of Advanced Materials Chemistry, Korea University, Sejong, Korea*

The catalytic efficacy of the mono-bipyridyl (η^6-*para*-Cymene)Ru(II) half-metallocene, $[(p\text{-Cym})Ru(bpy)Cl]^+$, was evaluated in both mixed homogeneous and heterogeneous hybrid system for photochemical CO_2 reduction. In homogeneous system, the conversion activity and product selectivity were impacted by the pK_a value and concentration of the proton source added. When a more acidic TEOA additive was introduced, the half-metallocene Ru(II) catalyst leaned toward producing formate (resulting in a $TON_{formate}$ of 784 and TON_{CO} of 130 over 48 hours). On the other hand, in homogeneous catalysis with TFE additive, the CO_2-to-formate conversion was less effective, yielding a more efficient CO_2-to-CO conversion with a selectivity of >80% ($TON_{formate}$ of 242 and TON_{CO} of 626 over 48 h). The preference between the two pathways was elucidated through an electrochemical mechanistic study. The TiO_2-heterogenized (*p*-Cym)Ru(II) catalyst demonstrated enhanced and enduring performance, attaining TONs of 1000 for CO_2-to-CO and 665 for CO_2-to-formate.

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Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

N-Heterocyclic Carbene Derived Radical Ligands for Metal Diradical Complexes

Subin Park, Dongmin Kang, Jeong-Yoon Hwang, Youngsuk Kim*

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N-Heterocyclic carbenes (NHCs) have been widely recognized for their ability to facilitate the generation and utilization of unstable species, including main group and organic radicals.[1-3] While stable organic and main-group radicals have been synthesized using NHCs, their potential application as radical ligands remain largely unexplored. Redox-active ligands, which can donate or accept electrons from substrate, are emerging as versatile participants in reactions with transition metal complexes, offering a wide range of physical properties and multi-electron transfer abilities.[4-6] Therefore, redox-active ligand chemistry has attracted significant attention not only within coordination chemistry research but also in catalysis and materials science. Our study reveals that NHCs combined with carbon disulfide (CS_2) form new redox-active ligands. We synthesized palladium complexes of these ligands, which exhibit ligand-centered diradicaloid properties. Notably, these complexes undergo ligand-centered two-electron oxidations, showcasing the redox-activity of NHC–CS_2 ligands.References1.*Chem. – Eur. J*. 2018, *24*, 19110.2.*J. Am. Chem. Soc*. 2021, *143*, 8527.3.*J. Am. Chem. Soc*. 2017, *139*, 15300.4.*Inorg. Chem*. 2011, *50*, 9737.5.*Chem. Soc. Rev*. 2013, *42*, 1440.6.*Eur. J. Inorg. Chem*. 2012, *2012*, 340.

Poster Presentation : **INOR.P-65**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of Novel Metal Clusters using Diamidocarbene–CS_2 Adduct

Minji Lee, Hyun Ju Noh, Youngsuk Kim*

Department of Chemistry, Pusan National University, Korea

Metal-sulfur clusters are highly versatile prosthetic groups found abundantly in nature, playing essential roles in various biological processes.[1–2] These clusters are typically associated with iron but may also incorporate other transition metals such as nickel, vanadium, or molybdenum. Due to their ability to facilitate even the most challenging catalytic reactions, many researchers are actively exploring novel metal-sulfur cluster compounds, incorporating diverse metals and ligands. In this study, we present the synthesis and detailed crystallographic characterization of two new metal-sulfur clusters, Pd_4S_8 and Ni_3S_8, utilizing the new DAC–CS_2 ligand derived from diamidocarbene (DAC) and carbon disulfide (CS_2).[3] These findings contribute to expanding our understanding of metal-sulfur cluster chemistry and offer new avenues for the synthesis of new metal-sulfur cluster with hitherto unknown connectivities.References1.*Coord. Chem. Rev.* 2022, *453*, 214229.2.*Nat. Chem.* 2022, *14*, 253.3.*J. Am. Chem. Soc.* 2009, *131*, 16039.

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Poster Presentation : **INOR.P-66**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Structure Analysis for Interpenetrated and Single-layered 2D Cu(II) Coordination Polymers

Eunbi Jeong, Haeri Lee*

Department of Chemistry, Hannam University, Korea

We successfully formed Cu(II) complexes, which crystal structures were analyzed single crystal X-ray diffractometer. Notably, the coordination environment and counter anions surrounding the Cu(II) ion played a pivotal role in determining the overall skeletal structure of the complexes. Our ongoing research focuses on further exploring the structural effects and implications of Cu(II) networks. By gaining a deeper understanding of these factors, we aim to enhance our knowledge of the properties and potential applications of copper-based coordination compounds. The reversible oxidation-reduction behavior of copper metal ions is a fascinating phenomenon with wide applications in the fields of catalysts and sensors. In our study, we aimed to construct coordination networks incorporating Cu(II) by designing and synthesizing a bis(monodentate) N-donor ligand. The ligand was thoroughly characterized using advanced spectroscopic techniques, including 1H, 13C, COSY NMR spectra, and mass spectrometry.

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Poster Presentation : **INOR.P-67**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Interfacial Engineering of Ru$_2$P/Ir$_2$P Heterostructure for Alkaline Hydrogen Evolution Catalysis with Efficient Hydrogen Spillover

Sangyeon Jeong, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

For hydrogen evolution reaction (HER) in alkaline media, a crucial consideration involves balancing hydrogen adsorption (H$_{ad}$), hydroxyl adsorption ((OH)$_{ad}$), and water dissociation. Therefore, designing electrocatalysts with exceptional capabilities in both water dissociation and binding hydrogen species emerges as a promising approach for crafting highly efficient alkaline HER catalysts. Despite the development of various single-phase catalysts for HER, many have struggled to overcome the inherent sluggish reaction kinetics in alkaline environments. Herein, we present the in-situ growth of Ir$_2$P clusters on R$_2$2P hollow nanotubes as highly efficient electrocatalysts for alkaline HER. Density functional theory calculations unveil that the distinctive geometrical features of protruded Ir$_2$P clusters on the surface of Ru$_2$P facilitate rapid cascade water dissociation and H$_2$ production. This is achieved by promoting hydrogen spillover from the Ru$_2$P surface to the adjacent Ir$_2$P cluster. This work highlights that rational synthesis of hybrid catalysts is a viable strategy for developing active and durable alkaline HER catalysts.

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Poster Presentation : **INOR.P-68**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Switching Properties of Zinc(II) Complexes

Sohyeon Kwon, Haeri Lee[*]

Department of Chemistry, Hannam University, Korea

Catalysts play a crucial role in enhancing the efficiency of chemical reactions in a field of environmental, industrial, and biological applications. In particular, heterogeneous catalysts provide the advantage of easy separation from the reaction solution. Polymeric metal compounds, which have less solubility in organic solvents, are applied as heterogeneous catalysts to initiate organic reactions.In this work, we synthesized discrete Zn(II)-based complexes and used them as catalysts in the transesterification reaction. The ligand and metal complexes were analyzed by spectroscopic techniques and characterized their crystal structures by X-ray diffraction method. Subsequently, the catalytic activities of these complexes in the transesterification reaction were examined. The use of halides, yields a series of [Zn2X4L] (X=Cl, Br, I) with low catalytic activity while Zn(ClO4)2 results in a [ZnL]n 1D coordination polymer with high catalytic activity. It show that polymer metal complexes significantly affect catalytic activity. So, Chemical stimuli that trigger anion exchange allows to switch on/off the systems' catalytic activity.

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Poster Presentation : **INOR.P-69**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Binder-Free Wrinkle-Multilayered Graphene Scaffold for Stable Lithium Metal Batteries

Sangyeop Kim, Won Cheol Yoo[1,*]

Department of Applied Chemisty, Hanyang University, Korea

[1]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

Lithium metal anodes (LMAs) with the highest theoretical capacity (3860 mAh g^{-1}) and low reduction potential (−3.04 V vs. standard hydrogen electrode) are the most promising candidates for batteries with high energy density. Nevertheless, the practical use of LMA is hindered by the high chemical reactivity of lithium and the infinite volume changes occurring during the plating and stripping processes. The scaffold/host design is recognized as the most effective method for simultaneously mitigating infinite volume changes and suppressing dendrite growth. Herein, wrinkled-multilayered graphene (WMG) is used as a host for the lithium metal batteries. The wrinkled morphology of WMG obviates the need for binders in electrode construction, while its mechanical properties and resilience afford resistance to volumetric changes. Consequently, lithium metal batteries incorporating WMG demonstrated improved rate capabilities and sustained long-term stability, crucial for the development of sophisticated electrochemical storage solutions.

Poster Presentation : **INOR.P-70**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Morphology tunable Fe@C for High-Performance Lithium Metal Batteries

InCheol Heo, Yejun Ham, Won Cheol Yoo[1,*]

Department of Applied chemistry, Hanyang University, Korea

[1]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

Lithium metal anodes offer high energy density due to their high theoretical capacity (3860 mAh g^{1}) and low reduction potential (-3.04 V vs. standard hydrogen electrode). However, lithium metal anodes face challenges such as uncontrolled lithium dendrite growth and infinite volume change. Host material design using carbonaceous materials is one of the strategies to address these issues. Herein, Urchin, Hollow Fe@C are used as a host for the lithium metal batteries. Hollow Fe@C exhibits lithiophilic surface and inhibition of Li dendrite formation based on size and morphology, resulting in reduction of dendrite formation and tolerance to the volume change. As a result, Hollow Fe@C-based lithium metal batteries showed outstanding rate performance and long-term stability essential for implementing advanced electrochemical storage systems.

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Inorganic Chemistry

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$FeSe_2$ Nanoparticles Coated with Graphitic Carbon for High-Capacity Potassium-Ion Battery Anodes

Boram Yun, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Lithium-ion batteries (LIBs) face challenges due to the increasing demands for energy storage, limited resources, and the high price of lithium. In response to the growing need for cost-effective energy storage solutions, potassium-ion batteries (PIBs) have emerged as promising candidates for the next generation of secondary batteries, owing to their low cost, abundant resources, and environmental friendliness. However, the large ionic radius of K^+ ions hinder their mobility, leading to slow charge and discharge rates and significant volume changes in the host material. In this study, we investigated $FeSe_2$ as a potential candidate for potassium-ion battery anodes due to its high capacity and stability. To address the challenges associated with K^+ ion mobility and volume changes, we coated $FeSe_2$ nanoparticles with graphitic carbon, synthesized from Fe-MIL-88B as a template. Our synthesized $FeSe_2$@2GC composite exhibited an enhanced discharge capacity of approximately 410 mAh g^{-1}, a significant improvement over bare $FeSe_2$ (110 mAh g^{-1}), after 250 cycles at a current density of 200 mA g^{-1} within a voltage range of 0.01 – 3 V.

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Poster Presentation : **INOR.P-72**

Inorganic Chemistry

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Morphology- and Crystallinity-Tunable Nickel Cobalt Oxide/Nickel Oxide Coated on Polypyrrole Electrode for Lithium-Ion Battery

Jaeseong Kim, Won Cheol Yoo[1,*]

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[1]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

In a recent study, the high demand for Lithium-Ion Batteries(LIBs) has high attention on the research of electrode materials that achieve high capacity and long-term stability. Nickel-cobalt-oxide (NCO) is a well-known Binary Metal Oxide (BMO) because of its higher theoretical capacity (890 mAh g-1 of $NiCo_2O_4$) and exceptional mechanical stability compared to single metal oxides like Nickel Oxide or Cobalt Oxides. However, its application has a challenging issue due to its volume expansion during charge-discharge cycles.In this study, we present easily morphology-controlled NCO into sea-urchin and flower form through hydrothermal synthesis using Ammonium fluoride (NH_4F) as a structural-directing agent. Furthermore, we coated polypyrrole(ppy) by Vapor-phase Polymerization method(VPP) as a conducting polymer to enhance its electrical conductivity. The morphology-controlled NCO@ppy provides large electrochemical active sites, excellently fast ion-diffusion during charge/discharge cycles, protects the structure from volume expansion, and improves electrical conductivity ensuring outstanding charge-discharge efficiency.

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Poster Presentation : **INOR.P-73**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Acrylate synthesis from ethylene and CO_2 using $(Cp^*)_2$Ti complexes

Areum Kim, Changho Yoo[*]

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

Carboxylation of ethylene using CO_2 is an attractive method for producing acrylic acid. The first catalytic synthesis of acrylic acid via ethylene carboxylation was reported in 2012 by the Limbach group. The obtained turnover number was merely 10 using nickel bisphosphine catalysts. Despite subsequent efforts employing group 10 metals, the highest TON reached was 514 with the $Pd(PPh_3)_4$/1,2-bis(dicyclohexylphosphino)ethane catalyst. Accordingly, exploration for superior catalytic system is imperative to enhance commercial viability. A metallalactone is a key intermediate for acrylate production from ethylene and CO_2. Despite the metallalactone formation is well documented with the early transition metals, their utilization in catalytic acrylate production is underexplored. We assumed that early transition metals deserve further investigation, as their vacant d orbitals can facilitate metallalactone formation by enhancing initial CO_2 coordination and stabilizing metal-oxygen bond through π interaction. In this study, we conducted stoichiometric and catalytic study of acrylate synthesis using $(Cp^*)_2$Ti complexes. The formation of titanalactone compound $(Cp^*)_2Ti(C_2H_4CO_2)$ was already reported, however, further reactivity study toward acrylate formation has never been evaluated. Optimization of titanalactone formation achieved 90% yield by minimizing possible side reactions. The subsequent reactivity study toward acrylate formation indicates strong titanium-oxygen bond suppresses β-hydride elimination. Direct deprotonation using an alkoxide base produced acrylate in 42% yield, but the use of strong base also resulted in a side reaction. Our study on the elementary steps offers insights and challenges for catalytic acrylate synthesis using early transition metals.

Poster Presentation : **INOR.P-74**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Rational Pore Design in Multivariate Metal-Organic Frameworks for C2H6/C2H4 Separation

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[1]Department of Chemistry & Nanoscience, Ewha Womans University, Korea

[2]Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The arrangement of pores within the framework plays a crucial role in the gas separation and adsorption of metal-organic frameworks (MOFs), determining their overall performance. In this study, we compare the impact on gas separation efficiency of two multivariate MOF (MTV-MOF) systems with controlled pore arrangements. These systems employ two types of ligands with differing bulkiness: one is the core-shell MOF composite (CSMOF), sequentially synthesized with the bulkier ligand located at the shell, and the other is the mixed-linker MOF (MLMOF), synthesized via a one-pot reaction. Interestingly, in MLMOFs, we confirmed that the distribution of bulky ligands increases gradually from the center to the surface, rather than being randomly distributed, forming a framework with finely tuned pores. MLMOF exhibited a high C2H6/C2H4 ideal adsorption solution theory (IAST) selectivity of over 2, attributed to the bulky alkoxy chain forming an overall contracted pore environment. Breakthrough experiments demonstrated the effective separation of C2H6/C2H4 in MLMOFs. This study indicates that maximizing performance depends on the specific partitioning of pore space in gas separations, and MTV-MOFs can be effectively applied in challenging gas separation scenarios.

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Enhancement in Photocatalytic Performance of PCN-222 via Incorporation of Heavy Metals and C60

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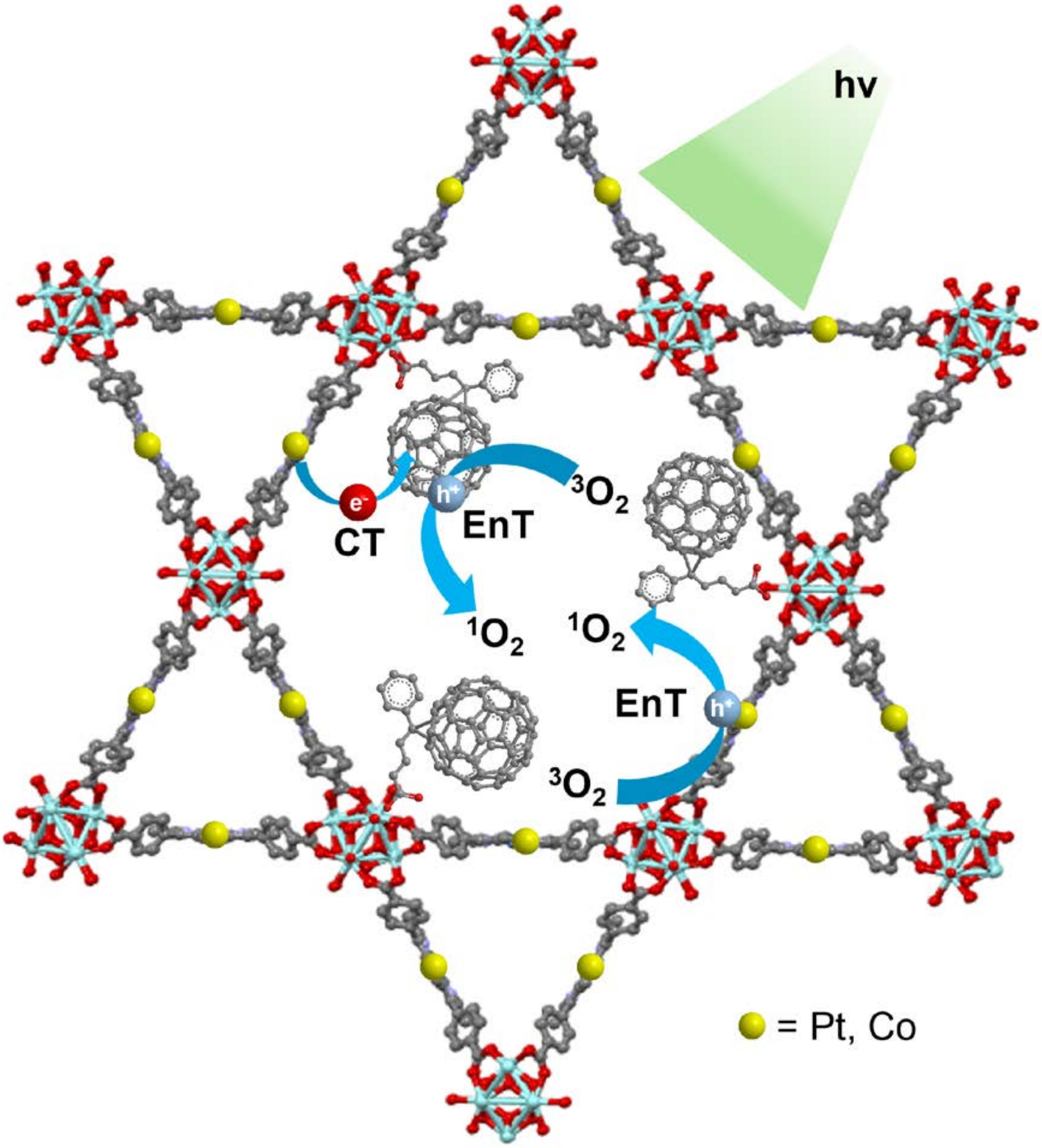
Department of Energy and Chemical Engineering, Incheon National University, Korea

Keywords: PCN-222, Heavy Atom Effect, Reactive Oxygen Species, C60, Energy TransferAbstract: Exploiting the light-induced energy transfer capabilities of metal-organic frameworks (MOFs) for generating reactive oxygen species (ROS) is a promising avenue in photodynamic therapy and photocatalytic oxidative reaction for environmental remediation. In this study, we explore the photosensitizing potential of PCN-222, a highly stable zirconium-based porphyrinic MOF, as an efficient platform for ROS generation through the incorporation of heavy metals (for e.g., platinum and cobalt) and fullerene (C60, which is a good electron acceptor). PCN-222 was synthesized as the host framework, and the controlled introduction of Pt and Co ions was carried out to enhance light absorption and facilitate efficient energy transfer. Concurrently, C60 was incorporated into the MOF matrix to serve as an electron acceptor, promoting charge separation and facilitating the generation of ROS.This study highlights the multifunctional role of PCN-222 as a platform for ROS generation through energy transfer by facilitating intersystem crossing to triplet state from incorporated heavy metals and electron transfer through C60. The synergistic effects of these components offer a novel strategy for developing MOF-based photosensitizers with enhanced efficiency for applications in photodynamic therapy and environmental pollutant degradation.


hν
e⁻
CT
h⁺
EnT
$^3O_2$
$^1O_2$
$^1O_2$
EnT
h⁺
$^3O_2$
= Pt, Co

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Poster Presentation : **INOR.P-76**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

High-Temperature Hydrogen Isotope Separation Enabled by Locally Flexible Gates in Tightly Confined Microporous Metal-Organic Frameworks

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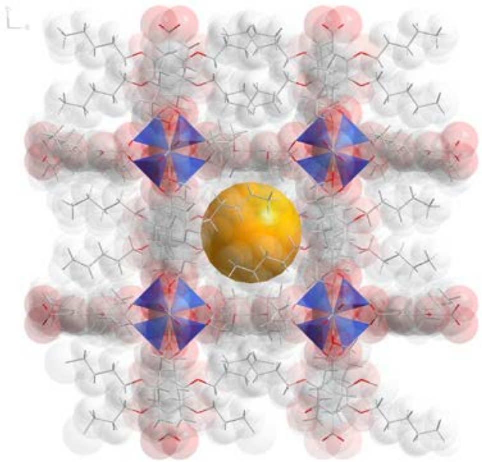
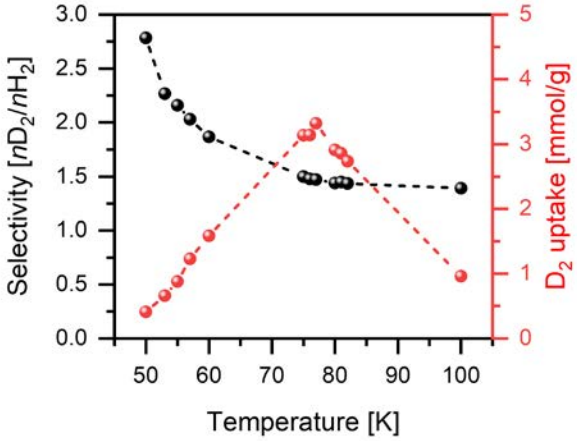
Deuterium separation from isotopic mixtures poses a significant challenge due to the nearly identical physicochemical properties of hydrogen isotopes. To overcome the low selectivity with low separation temperature of traditional separation methods, kinetic quantum sieving (KQS) has been proposed as an alternative concept. Metal-organic frameworks (MOFs) with their tunable pore have been prominent to provide the confined space for KQS, thus rigid MOFs with pore apertures of 3–3.4 Å have been widely studied. However, due to their weak binding energies on the outer surface of materials, the high performance only achieved at near the liquefaction temperature (20 K) of hydrogen. Several studies have demonstrated that introducing local flexibility into MOFs can create pore aperture sizes to closely match those of hydrogen isotopes at specific temperatures. This flexible gating provides effective diffusion barriers for hydrogen, enabling efficient separation at high temperatures above 70 K, thought only achievable with strong binding sites in pores. Such researches highlight the role of locally flexible gates at the apertures for achieving high separation temperatures. In this study, we aim to achieve high operational temperatures with large D_2 uptake by introducing bulky substituents functionalized linkers as locally flexible kinetic barriers in a series of isoreticular MOFs having large cavities, to achieve higher separation temperatures. Their kinetic behavior was analyzed using hydrogen sorption measurements and thermal desorption spectroscopy. Among them, C5-IRMOF exhibited the most effective confinement phenomenon for KQS at a significantly higher temperature of 100 K, with meaningful selectivity and a D_2 uptake of approximately 1.0 mmol/g.





Selectivity [nD_2/nH_2]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
50
60
70
80
90
100
Temperature [K]
D_2 uptake [mmol/g]
5
4
3
2
1
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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **INOR.P-77**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

FeOF Embedded in Graphitic Carbon as a High-Performance Cathode Material for Potassium-Ion Batteries

Ayesha Qayyum, Jongsik Kim[*]

Department of Chemistry, Dong-A University, Korea

Potassium ion batteries (KIBs) are promising alternative candidates for large scale energy storage because of their abundant availability, low cost, sustainability, long lifespan, high theoretical energy density, the low standard reduction potential of potassium, and fascinating K^+ transport kinetics in the electrolyte and their intercalation mechanism, which is identical that of lithium-ion batteries. Iron oxyfluoride (FeOF) is an appealing conversion type cathode material due to its low cost, eco-friendly, and relatively large theoretical capacity of 885 mAh g^{-1}. However, FeOF cathode has low rate and cyclability due to its low electrical conductivity and poor ionic diffusion coefficient. In this work, for the first time, carbon wrapped FeOF nanocomposite was synthesized by facile polymerization method with citric acid as both chelating agent and carbon source, and ethylene glycol as a cross linker. FeOF nanoparticle with conductive carbon shown excellent electrochemical performance in KIBs as compared to bare FeOF with a discharge capacity of 132.6 mAh g^{-1} and a fading rate of 0.21% after 200 cycles at 100 mA g^{-1} current density in a 1.2-4.0 V voltage range.

Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

RuO_2 Supported on the PtNi multi-frame for Enhanced Electrocatalytic Performance for Oxygen Evolution Reaction in Acidic Media

Doyeop Kim, Kwangyeol Lee[*]

Department of Chemistry, Korea University, Korea

The electrochemical process of water-splitting has attracted significant attention as a viable method for producing and storing 'green hydrogen.' This approach provides a robust, carbon-free means of hydrogen generation, substantially reducing reliance on fossil fuels. However, a key obstacle to improving the efficiency of this process is the sluggish kinetics of the oxygen evolution reaction (OER), especially in acidic electrolytes. The OER demonstrates a relatively slow reaction rate compared to the hydrogen evolution reaction (HER), mainly attributable to its 4- electron mechanism. Existing catalysts based on Ru nanoparticles show remarkable activity for acidic OER but are susceptible to dissolution in acidic conditions, limiting their stability. To address this issue, we have developed a novel approach to synthesizing RuO_2 catalysts supported by PtNi multi-frames. This involved a seed-mediated growth method followed by thermal oxidation, stabilizing the Ru-based nanocatalyst. Through temperature control of thermal oxidation, it is possible to adjust the degree of doping of Pt into RuO_2, and the migration of Ni and RuO_2 affects the OER performance, leading to exceptional catalytic activity and remarkable stability for the acidic OER. This study suggests an ideal synthesis method for efficiently introducing dopants into RuO_2-based catalysts and atomic migration while providing a new understanding of catalyst development with improved performance in acidic conditions for the OER.

Poster Presentation : **INOR.P-79**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Photoluminescence Properties of Bisquinoline Copper Iodide Complexes

Eun su Chae, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Photoluminescent materials can be applied for bioimaging, sensors, and LEDs. Copper iodide complexes with structural diversities often show photoluminescent properties which are potential for such applications. However, successful applications depend on the stabilities of the copper complexes in air. In this study, we synthesized air-stable monovalent and divalent copper iodide complexes with bisquinoline Schiff-base ligands. Two monovalent copper iodide complexes were found to be 1-D coordination polymers with Cu_2I_2 cores. In this poster, we discuss the synthesis, structure, and photoluminescent properties of the complexes.

Poster Presentation : **INOR.P-80**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

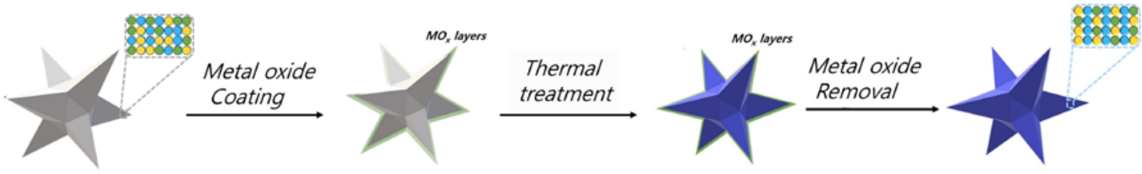
Platinum-based Ternary Intermetallic Hexapod Nanocatalysts for Oxygen Reduction Reactions

Seungjin Lee, Kwangyeol Lee[1,*]

Department of chemistry, Korea University, Korea

[1]Department of Chemistry, Korea University, Korea

Fuel cells, a promising technology in sustainable energy conversion systems, face challenges in commercial applications due to the slow kinetics of the oxygen reduction reaction (ORR) due to the complex mechanism dealing with 4 electrons. Therefore, effective electrocatalysts to accelerate the reaction are required. While platinum-based catalysts have impressive initial activities, their practical application in fuel cell devices is hampered by low durability due to non-platinum element dissolution during electrocatalysis. Herein, we present a novel method for producing platinum-based ternary intermetallic nanohexapods as ORR electrocatalysts. The high-index facets of the hexapod-shaped platinum-based intermetallic nanocatalysts are expected to reduce the absorption energy of reaction intermediates, resulting in high ORR catalytic performance. Furthermore, the intermetallic phase's stability due to the strong d-d orbital interaction would improve the catalysts' durability under harsh conditions. Hence, the platinum-based ternary intermetallic hexapod nanoparticle synthesized would lead to better ORR activity and durability.



Poster Presentation : **INOR.P-81**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Metal substitutability within the zinc finger domain and its regulatory role in dopamine release

Yunha Hwang, Dong-Heon Lee, Seung Jae Lee[*]

Department of Chemistry and Institute of Molecular Biology and Genetics, Jeonbuk National University, Korea

The major transcriptional and translational regulators in eukaryotes and prokaryotes are zinc finger (ZF) proteins. The structural and functional aspects of these proteins have been intensively investigated, owing to their crucial importance in the Central Dogma. ZF proteins have a distinct feature as metalloproteins, because the specific secondary folding in local ZF domains is generated in the presence of zinc ions. ZF domains consisting of Cys and His residues can function independently in many cases, and the biochemical aspects of these ZF domains are widely studied, to understand their specific roles. This presentation demonstrates the possible application of zinc fingers for recycling of metal ions, to obtain selective cobalt ions using induced *E. coli* systems. There have been precedent approaches that have attempted to understand the coordination of heterometal ions such as ferrous, ferric, cobalt, copper, and others through purified zinc finger domains, but this study provides possible applications of zinc fingers in biological systems. A classical three-zinc finger domains from the protein expressed in the brain was investigated to understand metal coordination. The results provided the valuable information that these domains selectively coordinate to cobalt in the *E. coli* system. Iron and copper cannot replace metal ions in PARIS, although iron improves the expression level of zinc-bound proteins. In addition, proteins were expressed and purified for basic characterization and showed cobalt-binding abilities.

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Poster Presentation : **INOR.P-82**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

The Fabrication of GaN-based Micro-light-emitting diode (LED) for Fluidic Self-assembly using Frequency Sonication

Yong Jae Lee, Huiyeong Kang, Sang Jun Kim, SeungJe Lee, Young rag Do*

Department of Chemistry, Kookmin University, Korea

This study investigates the production process of GaN-based micro-LED arrays and LED chips. Then, the procedure for transferring the manufactured micro-LEDs using the fluidic self-assembly method was explained. Technologies utilized for Micro LED transfer, including roll-to-roll, laser, and pick and place, exhibit thermal, mechanical, and chemical stability drawbacks. In addition, these methods are expensive to invest in upfront, time-consuming, and unsuitable for mass transfer. The advantages of utilizing Fluidic Self-Assembly (FSA) for transferring Micro LEDs include relatively low cost, high precision, and the ability to create versatile Micro LED arrays with various shapes of materials. Micro LEDs developed in this study are designed in a trapezoidal form consisting of C_2 and C_1 axes and can be transmitted in only one direction using FSA and sound wave energy. The manufacturing process involves growing GaN layers on 4-inch patterned sapphire substrates (PSS), which are then deposited with Indium Tin Oxide (ITO). In sequence, lateral LED arrays are fabricated through a series of steps involving photolithography, etching, and deposition techniques. The micro-LEDs, individually separated by blade dicing, are transferred onto Si cartridges using fluidic self-assembly techniques accompanied by low-frequency sound wave energy. It is envisaged that properly aligned GaN-based LED chips, utilizing appropriate transfer methodologies, will find wide-ranging applications in the display industry.

Poster Presentation : **INOR.P-83**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Transcriptional regulation via interaction between transcription factors and nucleic acid in soluble methane monooxygenase

Yunha Hwang, Dong-Heon Lee, Seung Jae Lee[*]

Department of Chemistry and Institute of Molecular Biology and Genetics, Jeonbuk National University, Korea

Methanotrophs play a role in regulating Earth's methane levels through the utilization of soluble methane monooxygenases (sMMO) and particulate methane monooxygenases (pMMO). However, the specific transcriptional regulatory mechanisms of sMMO and pMMO have not yet been fully elucidated. The sigma factor is essential for the transcriptional initiation. However, unlike sigma-70, sigma-54 relies on an enhancer-binding protein for transcriptional regulation. It has been proposed that MmoR may function as such an enhancer-binding protein in the transcriptional regulation of sMMO. We were successfully overexpressed MmoR and sigma-54 from *Methylosinus sporium* 5 in *Escherichia coli* and purified to investigate transcriptional regulation of sMMO in methanotrophs. Biophysical studies with fluorescence anisotropy have proved the promoter elements of type II methanotrophs positioned between *mmoG* and *mmoX1*. This transcriptional process is initiated through the involvement of adenosine triphosphate (ATP), as it facilitates the interaction between the enhancer-binding protein and the sigma factor. The upstream activating sequences (UAS) are generally positioned -80 to -160 from the transcriptional start site. We were able to identify commonly identified UAS sequences (ACA-xx-TGT) through sequence alignment of the methanotroph superfamily. MmoR exhibits a strong binding affinity ($K_d = 12.5 \pm 0.5$ nM) for the UAS in its interactions. The experiments of titration revealed that MmoR did not directly bind with copper ions. However, the binding affinity of MmoR to UAS is decreased by increasing the concentration of copper ions. This research demonstrated that the binding interactions of both MmoR and σ^{54} that regulate transcription of sMMO and pMMO in *M. sporium* 5 depend on the Cu ion concentration.

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Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Enhanced Face-Selective Assembly of Dot-LEDs via Au-Dithiol-Au Bridge Linker

Soyeon Kim, Yeong Been Oh, Yujeong Jeong, Minji Ko, Young rag Do[*]

Department of Chemistry, Kookmin University, Korea

MicroLED displays are gaining attention as next-generation display technology due to their extended lifespan and higher brightness than OLED displays. The commercialization of Micro-LED technology faces a challenge during the mass transfer process, which involves efficiently transferring Micro-LED chips from fabrication wafers to displays.In this study, we utilized self-assembled monolayers (SAMs) of thiols on gold surfaces as the binding method to transfer Cr/Au Dot LEDs onto the gold electrode. Due to their rapid evaporation rate, LEDs dispersed in acetone ink Indicate a low p-contact ratio. Polyethylene Glycol (PEG) acetone mixed solvent increases surface tension and the reaction time between gold (Au) and thiol. Additionally, we investigated the effect of enhancing LED selective assembly on the contact rate based on the variables of SAM concentration (0.1, 0.5, 1, 5, and 10 mM). Different from expectation, nanoscale GaN-based dot light-emitting diode (LED) displays with diameters of 1350 nm and height of 1550nm were assembled by only 25% when acetone was used. The assembly yield was significantly increased to 70% when a PEG-acetone mixed solvent was used due to the control of both vapor pressure and surface energy of the mixed solvent.The precise and stable bonding between Au electrodes and dithiols of LEDs enhances pixel assembly, allowing for high-resolution and high-quality displays. The resolution of mass transfer issues in Micro-LED technology is expected to promote the possibility of the successful commercialization of the technology.

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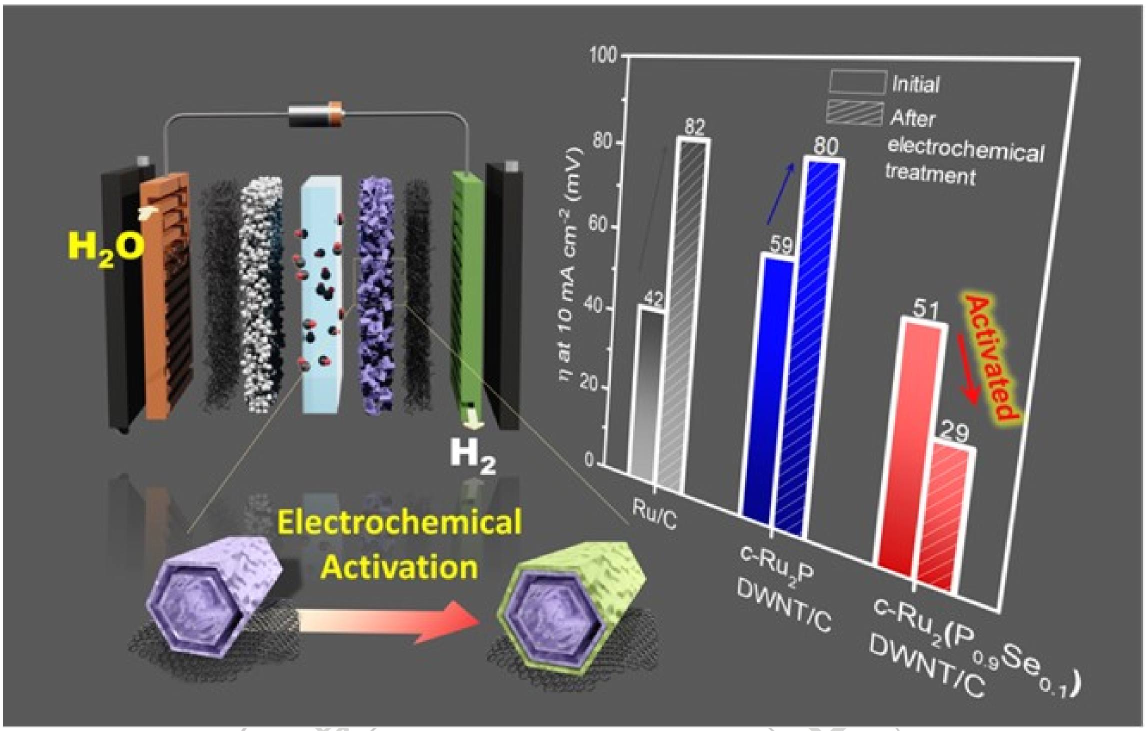
Poster Presentation : **INOR.P-85**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Engineering the Electronic Structure of Ruthenium Phosphide via Selenium Doping for Alkaline Hydrogen Evolution Reaction

Eunsoo Lee, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Hydrogen(H_2) generation via electrocatalytic reduction of water is a promising technology that can provide sustainable and eco-friendly energy. However, the hydrogen evolution reaction (HER) in alkaline conditions remains challenging because of its sluggish reaction kinetics due to the additional water dissociation step. Herein, we synthesize Se-doped Ru_2P double-walled nanotube catalyst via alternating anion and cation exchange reactions of $Cu_{1.8}S$ hexagonal nanorod templates. It also demonstrated outstanding catalytic activity and durability toward alkaline HER after electrochemical priming, with low overpotential of 29 mV at 10 mA cm^{-2}. We investigated the evolution of Ru-OH moiety thorough X-ray spectroscopy, which provides strengths for catalytic properties on the Se-modulated catalyst. Experimental and theoretical calculation results revealed that the surface doped Se leads advanced structural stability of the intermediately formed active Ru-OH species, and its suitably modified electronic structures. Furthermore, the outcome of an anion-exchange membrane water electrolyzer (AEMWE) performance and MD simulation with Se-Ru_2P catalyst revealed that the incorporated Se on Ru_2P surface elevated the water penetration in electrode-electrolyte interface.


H2O
H2
Electrochemical Activation
100
80
60
40
20
0
η at 10 mA cm-2 (mV)
Initial
After electrochemical treatment
42
82
59
80
51
29
Activated
Ru/C
c-Ru2P DWNT/C
c-Ru2(P0.9Se0.1) DWNT/C

Poster Presentation : **INOR.P-86**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

The Fabrication of Dot-LED Electroluminescent Device Using ~ 1μm Scale Dot-LED Ink

Yujeong Jeong, Soyeon Kim, Heemin Oh, Minji Ko, Young rag Do*

Department of Chemistry, Kookmin University, Korea

Micro light-emitting diodes (LEDs) achieve high luminous efficiency and stability but have high production costs. To reduce the cost of micro-LED, scaling down LED size from micro to nanoscale can substantially decrease material cost per pixel.In this research, we fabricated nanoscale dot LEDs as an alternative to micro-LEDs and applied them to an electroluminescent (EL) device. The dot LEDs with a diameter of 1.05 um and a height of 1.25 um were fabricated using the top-down approach. The dot LEDs were separated through electrochemical etching (ECE) and sonication by selecting the ink based on low vapor pressure. The self-assembled monolayers (SAMs) method achieved vertical assembly on the electrode. The fabricated EL device has a peak external quantum efficiency (EQE) of 6.3% at an applied voltage of 3.0 V and luminance of 2530 cd/m2 at an applied voltage of 8.0 V. To be applied in augmented reality (AR)/virtual reality (VR) display industry, a smaller size with a higher pixels per inch (PPI) is necessary. By fabricating the ~1μm scale dot-LED EL device, we show its potential to become a new-generation display.

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Poster Presentation : **INOR.P-87**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Facile Cleavage of O=S and N=S Bonds by Diamidocarbene

Hyunju Noh, Youngsuk Kim[1,*]

Pusan National University, Korea

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

N-heterocyclic carbenes (NHCs) are famous ligands known for forming stable complexes with various transition metals due to their strong σ-donating abilities. Recent studies show their capability to activate small molecules, mimicking the chemical reactivity of transition metal centers, attributed to their lone pair of electrons and accessible empty orbital. Notably, diamidocarbene (DAC), an NHC with strong electrophilicity, exhibit reactivity with various small molecules such as alkenes, aldehydes, alkynes, nitriles, and isonitriles, resulting in the cleavage of various chemical bonds. Here we report that DAC can activate O=S and N=S bonds. Cleavage of double bonds is a challenging four-electron process that is rarely observed even for transition metal centers. The reaction between DAC and sulfur dioxide (SO_2) resulted in the complete cleavage of S=O bond, yielding DAC=O and DAC=SO species. We provide crystallographic characterization of DAC=SO and discuss the mechanism of its formation.

Poster Presentation : **INOR.P-88**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Improving Stability and Efficiency of Quantum Dots for Color-by-Blue Displays Using QD-embedded Alumina Microbeads

Jun Hwan Oh, Hansol Lee, Yeong Been Oh, Minji Ko, Young rag Do[*]

Department of Chemistry, Kookmin University, Korea

OLED advancements have led to the emergence of QLEDs in displays, offering easy color tuning, high PL quantum yield, and a narrow emission spectrum. InP/ZnSeS/ZnS quantum dots, with exceptional optical performance, have gained attention for low toxicity and cost-effectiveness. However, methods to address optical challenges in transitioning QD nanoparticles to QD films are underdeveloped. Films incorporating InP/ZnSeS/ZnS quantum dots within microbeads have been successfully engineered, resulting in improved scattering effects, operational stability, and luminous efficacy (LE). The three-step protective approach involves the introduction of aluminum (Al) dopant to rectify shell defects, the use of Hf-n-butoxide (Hf(OtBu)4)-complex treatment to reduce ligand detachment, and the application of an Aluminum tri-sec-butoxide (Al(OsBu)3) electrospray (E-spray) technique. This process creates an outer protective layer, transforming the material into Al2O3 microbeads embedded with quantum dots (QDs). Including Al dopant and Hf-alkoxide-complex techniques enhances carbon quantum dots' stability and photoluminescence quantum yield (PLQY) (C-QDs). This makes them suitable for embedding Al2O3 microbeads, minimizing PLQY and stability loss during the rapid hydrolysis E-spray process using Al(OsBu)3 precursor. Thus, the developed remote-type QD-emissive films, incorporating a mix of QD nanoparticles and microbeads, attain outstanding color purity, luminous efficacy (LE), and improved photo- and thermal stability. The mixed film plays a dual role as a QD-emissive and scattering material featuring QD microbeads. This is a proof-of-concept study on QD-OLEDs or QD-LEDs to explore the ideal composite structure for highly efficient and stable green color in color-by-blue QD displays.

Poster Presentation : **INOR.P-89**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Fabrication and Separation of GaN-Based Nano-LEDs via Electrochemical Etching

Yuna Kwon, Yong Jae Lee, Sang Jun Kim, Huiyeong Kang, SeungJe Lee, Young rag Do[*]

Department of Chemistry, Kookmin University, Korea

Currently dominating the display market, OLEDs have the disadvantage of being vulnerable to moisture and oxygen because they are based on organic materials. Therefore, inorganic micro- and nano-LED displays, overcoming OLED drawbacks, are gaining attention as next-generation displays with high efficiency and low power consumption. The Laser Lift-Off (LLO) method, known for separating micro-scale LEDs, employs a beam to detach LED chips from the wafer. However, getting nano-sized GaN LED chips from a wafer using the usual LLO method may lead to chip losses. Due to the small size of LEDs, developing a substrate separation process is essential to minimize losses and ensure efficient nano-sized LED chips.In this study, we introduced a novel electrochemical etching (ECE) process to separate the nanoscale LEDs from the wafer. Hole generation at the interface, oxidation of semiconductor surface, and then oxide dissolution in the electrolytes. Through this mechanism of anodic etching, n-GaN is porously and selectively etched. Subsequently, nanoscale LEDs were separated using a sonicator to induce cavitation effects. Etching was conducted regularly, varying the voltage from 7V to 15V. Voltage-dependent trends were observed, with etching depth increasing as the voltage increased. The impact on quantum well (MQW) structures and defects were assessed through photoluminescence and Raman spectroscopy. The effect of voltage on the n-GaN surface was confirmed by Atomic Force Microscopy (AFM). Using a scanning electron microscope (SEM), the degree of separation was examined for each voltage variable, determining optimized etching conditions. This study introduces a simple method to separate nano-sized LEDs from a wafer. These findings have considerable significance for researchers focused on enhancing the efficiency of nanoscale LED devices, optimizing future LED structures, and pioneering new fabrication methods and materials in the ultrasmall LED display industry.

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Poster Presentation : **INOR.P-90**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

The Fabrication of Multi-Layered Axial Heterostructure Nanorods for Modulating Polariton Lasing via Gain Volume Control

Huiyeong Kang, Yuna Kwon, SeungJe Lee, Minji Ko, Young rag Do*

Department of Chemistry, Kookmin University, Korea

The fabrication of nanorods featuring a multilayered axial heterostructure was initiated to facilitate polariton lasing. The main objective was fabricating a nanorod laser to stimulate polariton lasing to obtain modifiable characteristics encompassing the lasing threshold, emitted light wavelength, and mode spacing. A bottom-up approach was employed to deposit multilayered thin films, involving precise layering of InGaN, GaN, and AlGaN films using the metal-organic chemical vapor deposition (MOCVD) technique. Then, a top-down process was performed to manufacture these nanorods using nanoimprinting and dry/wet etching processes, resulting in a precisely stacked structure. GaN nanorods with flat ends were carefully engineered to attain nearly consistent measurements (~3μm length, ~500nm diameter).Variations in amplification efficiency and charge carrier transfer resulted in distinct lasing characteristics within the heterostructure. By adjusting layer thickness, tuning of mode spacing was achieved, as polaritons experienced differing refractive indices in different layers. The enhanced effective refractive index of GaN amplified the contrast at the interfaces between layers, resulting in enhanced reflectivity and a decreased lasing threshold—unique Fabry-Perot lasing modes allowed for adjustable mode spacing by manipulating polaritonic effects and composite materials. Adding silver thin films (~10nm) on the end surfaces enhanced reflectivity, providing a means to regulate the lasing threshold. The groundbreaking identification of polariton lasing in a multilayered axial heterostructure nanorod underscores the capacity to control lasing properties by adjusting gain volume, layer arrangement, and end facet configuration. The lasing results obtained indicate that the fabricated nanorod lasers, produced through intricate top-down processes, closely match the intended design structure. Consequently, the polariton lasing observed, featuring a varied spectrum within the multilayered heterostructure, underscores the potential for creating nanorods with a complex axial heterostructure, combining bottom-up multilayer growth and top-down fabrication approaches per the design specifications—the fabrication of versatile nanorod lasers with polariton lasing exhibit promising prospects for producing highly complicated nanoscale devices.

Poster Presentation : **INOR.P-91**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Removal of Aqueous Phenolic Contaminants using Metal-Organic Framework

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

Global climate change is worsening due to changes in pollutant concentrations, and extreme weather circumstances are occurring frequently. Among the various substances that pollute water, phenolic contaminants are one of the targets that must be removed as they harm humans and the ecosystem. Phenol-based compounds are highly toxic and biological recurrent carcinogenic contaminants even at low concentrations, so they must be removed. In the past, phenol-based compounds were removed through Cl^- ion, providing an H-bond acceptor site for the -OH group in phenol. However, these chlorinated chemicals produce aqueous Cl^- which may corrode iron. Following that reason, many researchers developed several technologies for removing the contaminants in aqueous. One of the removal methods, adsorption-based technologies using metal-organic frameworks (MOFs) are the most employed method to treat phenol compounds. MOFs are porous materials composed of metal clusters and organic ligands. In this work, two Zr-based MOFs, UiO-66 and UiO-67, which are structurally stable and have a high specific surface area, were synthesized. After MOF was loaded on phenolic contaminants prepared using water as a solvent, UV-vis analysis was performed, and the degree of adsorption according to the change in absorbance could be determined. This study can be expected to be highly effective in adsorbing and removing phenolic contaminants. Further research is progressing on the contribution of MOFs depending on the type of contaminant.

Poster Presentation : **INOR.P-92**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Nanosphere ZnSe-rGO as Anodes for Sodium-ion Batteries: mechanism study

Youngho Jin, Yoon Myung[1], Chan Woong Na[1], Jaewon Choi*

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[1]*Korea Institute of Industrial Technology, Korea*

Metal selenide have gained significant attention as suitable anode materials due to their redox potential range and high capacity. Among them, zinc selenide (ZnSe) has been widely recognized as a potential anode material for sodium-ion batteries (SIBs) with its variable application. Nevertheless, its poor electronic conductivity and volume variation remain as challenges for practical application. In this study, we seek to overcome the limitations of ZnSe by compositing ZnSe with reduced graphene oxide (rGO). Our approach involves synthesis of nano-sized materials and growing ZnSe on the surface of rGO (ZnSe-rGO). The morphology and properties of ZnSe and ZnSe-rGO are characterized using scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD). The sodium-ion storage of ZnSe is investigated using cyclic voltammetry, galvanostatic charge/discharge testing, ex situ X-ray diffraction and in situ X-ray diffraction. Conversion reaction during the several discharge processes is identified by analyzing the CV curves and results of X-ray diffraction data. ZnSe-rGO exhibits a cycle performance (discharge capacity of 316.1 $mAhg^{-1}$ at a current density of 0.5 Ag^{-1} after 1000 cycles). This study allows us to shed light on the charge/discharge mechanism of ZnSe, demonstrating that ZnSe-rGO is a suitable anode material for SIBs.

Poster Presentation : **INOR.P-93**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

A Study on the Lithiation Mechanism of Perylene Diimide with 3-Triazole Ring as an Organic Cathode for Lithium-Ion Batteries

Honggyu Seong, Yoon Myung[1], Chan Woong Na[1], Jaewon Choi[*]

Department of Chemistry, Gyeongsang National University, Korea
[1]*Korea Institute of Industrial Technology, Korea*

Organic compounds have a lot of advantages such as eco-friendly properties and abundant and cheap elements (C, H, O, N, etc.) from various resources compared to inorganic-based materials. Due to these features, they have been widely recognized as new cathode materials for lithium-ion batteries (LIBs). In this work, perylene diimide with 3-triazole ring (PDI-3AT) was synthesized via simple one-step condensation reaction. PDI-3AT revealed the reversible redox behavior in LIBs system. Furthermore, PDI_3AT delivered the excellent cycle performances of 100th discharge capacity of 85.2 mAh g^{-1} (@50 mA g^{-1}) and 1000th discharge capacity of 64.5 mAh g^{-1} (@500 mA g^{-1}). The mechanism of lithiation and de-lithiation processes was studied by ex-situ XPS and ATR FT-IR analyses of charged and discharged PDI-3AT cathodes, and DFT-based calculations. Also, it showed that improvements of lithium-ion diffusion coefficient and charge-transfer resistance were related with phase transition of PDI-3AT during the initial cycles. These results are expected to give an insight into the development of perylene-diimide-based organic cathodes materials.

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Improved Isolation Performance of Exosomes from Bovine Milk Using Electrophoretic Oscillation-Enhanced Tangent Flow-Driven Ultrafiltration

Hansol Lee, Jun Hwan Oh, Heemin Oh, Sang Jun Kim, Minji Ko, Young rag Do*

Department of Chemistry, Kookmin University, Korea

Exosomes, a type of extracellular vesicle, are versatile carriers with promising diagnostics, therapy, and skincare applications. They facilitate intercellular communication and hold potential for targeted drug delivery and disease diagnosis. The tangent flow-driven ultrafiltration (TF-DU) technique is gaining prominence for economically and efficiently isolating exosomes compared to conventional ultracentrifugation methods. Using atomic layer deposition (ALD), Al2O3 was deposited onto SiNx nanofilter membranes to adjust the pore size to match the size of exosomes (50 nm - 150 nm), enabling efficient separation of exosomes from bovine milk in their native form. However, the application of TF-DU faces challenges, such as nanopore clogging from larger EVs and milk proteins and forming a cake-like layer. Electrophoretic oscillation (EPO) was integrated into the TF-DU method to overcome these challenges. This advanced approach enhances filtration efficiency by removing larger EVs and aggregated proteins from the filter pores. By varying voltage and frequency during filtration, obtaining more than double the amount of filtrated milk under optimal conditions compared to using TF-DU alone was possible. Through the synergistic use of EPO and TF-DU, the nanopore blockage caused by larger milk-derived substances has been effectively addressed for over seven days. The separated particles were confirmed to be exosomes through various methods, and exosomes isolated using the EPO-enhanced TF-DU method measured 89.7 nm in size via nanoparticle tracking analysis (NTA). This innovation offers significant potential for refining the purification of exosomes from complex biological matrices and will open possibilities for research utilizing exosomes across numerous application areas.

Poster Presentation : **INOR.P-95**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

A new strategy for synthesis of Sb_2Se_3@MWCNT as high-stability anode for SIBs

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department of chemistry, Gyeongsang National University, Korea
[1]*Korea Institute of Industrial Technology, Korea*
[2]*Department of Chemistry, Gyeongsang National University, Korea*

Metal chalcogenides are considered as promising electrode for sodium-ion batteries (SIBs). Among them, Antimony selenide (Sb_2Se_3) is an attractive anode material due to low cost and high theoretical capacity. In addition to Sb_2Se_3, carbon nanotubes (CNTs) with high conductivity have been used as additives. In this work, we synthesized Sb_2Se_3@MWCNT nano-compounds (NCs) via one-step composite process and executed electrochemical performance as an anode for SIBs. Sb_2Se_3@MWCNT NCs exhibited improved capacity at 100 mA g^{-1}, and excellent cycle stability at 500 mA g^{-1} in comparison to Bare Sb_2Se_3. MWCNTs showed reduced charge-transfer resistance (Rct of 2.7Ω for Sb_2Se_3@MWCNT against 184Ω for Bare Sb_2Se_3) in Electrochemical impedance spectroscopy (EIS) measurements.

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Poster Presentation : **INOR.P-96**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Modulating photophysical properties of phosphorescent complexes by the electro-inductive effect

Eunji Lee, Mu-Hyun Baik[1,*]

Korea Advanced Institute of Science and Technology, Korea

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In 2020, our group reported the electro-inductive effect (EIE), that the electrode in an electrochemical apparatus behaves as a functional group and modulates the electronic properties and reactivities of the attached organic molecules.[1] By utilizing EIE, we envisaged that the electronic and photophysical properties of the phosphorescent materials can be controlled. To control the light-emitting properties, different dopants bearing distinct electronic properties need to be synthesized and analyzed. The electro-inductive effect, on the other hand, offers a novel approach to modulating the photophysical properties of the dopant without laborious synthetic difficulties. Moreover, one can control the color profile in a continuous manner, which is not viable using traditional synthetic approaches. In this study, we demonstrate how the photophysical properties of Iridium complexes can be changed through the electro-inductive effect. The excited state behavior of the dopant is studied both experimentally and computationally.

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Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Porous Aromatic Framework 41 as sulfur Support for High Performance Lithium Sulfur Batteries

Qian Wang, Ji Man Kim*

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In recent years, lithium-sulfur (Li-S) battery has attracted tremendous attention due to the low cost, environmental benignity, high energy density. Despite of the high energy density, the intrinsic features of poor conductivity, high capacity decay, self-discharge inhibit the application of Li-S battery. A key problem is the shuttle effect that induced by the dissolved lithium polysulfides. Hunting suitable sulfur support is presently well-known an effect route to mitigate shuttle effect. Porous organic frameworks (POFs) feature in designable structure and composition, large surface area, tunable pore size, high thermal and chemical stability, and ready functionality. These characteristics render POFs promising sulfur support in Li-S battery. Here, N-containing porous aromatic framework of PAF-41 is synthesized and directly used as the sulfur support without any post treatment. SPAF-41 composites were prepared by melt-diffusion strategy. The SPAF-41 electrode with high sulfur loading of 72 wt.% delivers a specific capacity of 725.8 mAh g^{-1} at 0.5 C at the first cycle. The sustained capacity of 491.4 mAh g^{-1} after 500 charge-discharge cycles at 0.5 C indicates an improved long-term cycling stability with a low decay rate of 0.06% per cycle.

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Poster Presentation : **INOR.P-98**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Facile Conversion from Achiral to Chiral Metal-Organic Framework for Asymmetric Catalysis

<u>Yera Jeong</u>, Younghu Son, Min Jeong Park, Minyoung Yoon[*]

Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea

Metal-organic frameworks (MOFs) are porous materials with high surface areas and easy tunability, making them versatile for applications in various fields such as gas separation, catalysis, and more. For introducing chiral functional groups into MOFs, methods commonly involve direct approaches and post-synthetic modifications. However, these methods face challenges, such as difficulties in synthesizing new chiral ligands. An alternative synthesis method, the synthesis of chiral MOF catalysts, can be facilitated using a technique called solvent-assisted ligand incorporation (SALI). In this study, L-proline was selected as a chiral catalytic moiety and incorporated into the framework of the stable MOF, UiO-66. To modulate the porosity and functionality (and thus performance) of UiO-66, a defect engineering technique was employed, which is involved in UiO-66 synthesis in the presence of a modulator, benzoic acid, to induce cluster defects. Subsequently, SALI was applied to the defective MOFs for the synthesis of chiral UiO-66 (UiO-66-L-proline). Due to the well-known catalytic activity of L-proline in an asymmetric aldol reaction, the prepared UiO-66-L-proline was used as a catalyst for aldol reactions. The catalytic activity of the MOF was compared with its homogeneous counterpart. In addition, the catalyst loading may affect the catalytic activity of the prepared MOF. These results may allow a facile preparation of an asymmetric catalyst for enantioselective catalytic reactions. Details of this work will be presented.

Poster Presentation : **INOR.P-99**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Selective Supramolecular Synthesis Strategy by Regulating Hydrogen Bonding between Pyrazole Ligands

Yeji Cha, Junseong Lee[*]

Department of Chemistry, Chonnam National University, Korea

Using hydrogen bonds to selectively form complexes is one of the strategies for supramolecular synthesis. Such complexes have high stability due to the assembly of supramolecules via hydrogen bonding. While there have been several reports on synthesizing supramolecules using different hydrogen bonding methods, research on controlling hydrogen bonding for the selective synthesis of supramolecules has been relatively scarce. Therefore, this study aims to address this gap by investigating a synthetic method that controls hydrogen bonding during the synthesis process to generate supramolecules selectively. Pyrazole, which contains two nitrogen atoms, is an ideal building block for supramolecular synthesis, as it easily forms hydrogen bonding of N-H···N. By carefully adjusting the reaction conditions, hydrogen atoms attached to nitrogen in pyrazole can be removed. This opens up new possibilities in generating supramolecules with selective hydrogen bonding, making pyrazole an excellent candidate for creating complex structures.

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Poster Presentation : **INOR.P-100**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Design of Cadmium Sulfide Nanoplatelets Deposited with Metal Cocatalyst and Their Photocatalytic Reaction

Yunkyoung Han, Hyunjoon Song*

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

Solar-to-energy conversion using semiconductor nanocatalysts represents a promising approach for sustainable clean energy production. Among numerous types of semiconductor photocatalysts, metal sulfide-based nanomaterials are being intensively studied due to their compatibility with visible light. Deposition of metal cocatalysts on metal sulfides to form metal-semiconductor hybrid structures has an advantage of improving carrier lifetime by transferring photogenerated electrons to the metal domains. Furthermore, introducing two-dimensional (2D) structure provides a larger absorption area and reduced carrier diffusion length to the surface, thus able to further enhance photocatalytic efficiency. Applying the aforementioned strategies, we synthesized 2D cadmium sulfide nanoplatelets (CdS NPLs) and introduced metal cocatalysts (Pt and Au) by varying deposition methods for photocatalytic platform. Under controlled reaction conditions, size and the number of metal cocatalysts on CdS NPLs could be successfully manipulated. We then investigated the photocatalytic reactivities of the prepared metal-CdS NPLs, including hydrogen evolution, carbon dioxide reduction, and lactic acid oxidation. This study envisions that the metal-CdS NPL hybrid nanostructures would be promising platform for versatile applications in photocatalytic reactions.

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Poster Presentation : **INOR.P-101**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Air-/Moisture-Stable Radical Pairs from 1,2-Dicarbonyl Radical Cation and TCNQ Radical Anion Derivatives

Sumin Kim, Sun Hee Kim[1,*], Jeongcheol Shin[2,*], Eunsung Lee[3]

Chemistry, Pohang University of Science and Technology, Korea
[1]*Western Seoul Center, Korea Basic Science Institute, Korea*
[2]*Department of Chemistry, Duksung Women's University, Korea*
[3]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Radical ion pairs composed of radical cations and radical anions have recently attracted much attention in the fields of catalysis and quantum information. However, few examples of their structures and properties have been reported since radical ion pairs are very unstable and highly reactive in air. Here, we report the synthesis and characterization of air- and moisture-stable radical pairs. They were synthesized from a simple salt metathesis reaction from 1,2-dicarbonyl radical stabilized by N-heterocyclic carbenes (NHCs) with NaTCNQ (Sodium Tetracyanoquinodimethane) and NaF_4TCNQ (Sodium 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane) . We have fully characterized the radical pairs including electron paramagnetic resonance (EPR) and single crystal X-ray diffraction (SCXRD). Both radical cation and radical anion are isolated in solid-state structures with minimal pi-pi stacking interaction. In addition, we performed Pulse EPR experiments to see if these radical pairs could be applied to qubits, the smallest unit of Quantum information processing (QIP). The T_1 relaxation time and T_2 relaxation time of the radical pair, which are related to the lifetime of the qubit, were measured and it was found that the $T_1$and T_2 relaxation times increased noticeably by forming a radical pair. Detailed characterizations will be presented.

Poster Presentation : **INOR.P-102**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Organotin Cluster Photoresists for Extreme Ultraviolet Lithography

Sihyun Woo, Jihye Baek[1], Youngmin You[1,*]

Chemical Engineering and Materials Science, Ewha Womans University, Korea
[1]*Chemical and Biomolecular Engineering, Yonsei University, Korea*

The demand for smaller electronic devices drives a shift in the semiconductor industry towards using extreme ultraviolet lithography (EUVL) for next-generation integrated circuits. Transition metal complexes, including those based on tin, have shown great promise as negative-tone photoresists in the field of EUVL. To harness their full potential for EUVL applications, it is crucial to enhance their EUV sensitivity, thermal and storage stability, and ease of processing. In pursuit of these goals, we developed eight organotin complexes with bis(pyrazolecarboxylate) as bidentate ligands, where two pyrazole rings are connected by varying alkyl chains. Our research revealed that the complex containing a propylene chain link demonstrated superior EUVL performances, successfully generating well-defined ~20 nm line/space patterns with an e-beam exposure of 1200 μC cm^{-2} or an EUV exposure of 221 mJ cm^{-2}.

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Poster Presentation : **INOR.P-103**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Metal-triggered supramolecular hydrogels based on bipyridine ligand possessing hydrazine moieties with metal ions

Kayeong Go, Sung Ho Jung*, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Bipyridine-based gelator 1 having two D-alanine units was prepared, and its gelation ability was evaluated in the presence of Co(NO3)2 and AgNO3 in water. Gelator 1 could gelate H2O in the presence of Co(NO3)2 or AgNO3 (1.0 equiv.) in water. Gelator 1 formed a 2:1 (1:Co2+) octahedral complex with Co2+, whereas it formed a 2:1 (1:Ag+) tetrahedral complex with Ag+. The metallosupramolecular hydrogel with Co2+ assembled into a left-handed helical fiber, whereas that with Ag+ assembled into a nanorod structure. 1H NMR and FTIR analyses revealed that π–π stacking and intermolecular hydrogen bonds acted as the driving force for the formation of the supramolecular nanoarchitectures. Furthermore, to characterize the viscoelastic properties of hydrogels, rheology experiments were conducted at 25C, including time, strain, and frequency sweeps.

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Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Emission control of supramolecular bimetallic gels

Eungyu Lee, Jong Hwa Jung*, Sung Ho Jung*

Department of Chemistry, Gyeongsang National University, Korea

We demonstrated that a terpyridine derivative 1 forms emissive supramolecular metallogels in a mixture of MeOH and H2O (v/v, 1/1) with lanthanide ions. The complex of lanthanide metal ions such as Tb(III) and Eu(III) ions with terpyridine ligand generated supramolecular metallogels emitting green and red fluorescence, respectively dye to energy transfer from the terpyridine moiety to the lanthanide ions. Furthermore, fine-tuning of the emission properties of the supramolecular metallogels was achieved by precisely controlling the molar ratio of 1:Tb:Eu during the formation of homogenously mixed gels. This resulted in supramolecular bimetallic gels with yellow and white luminescence properties. The supramolecular metallogels were characterized through UV/Vis spectroscopy, fluorescence spectroscopy, scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDXS), and CIE color coordinates. This study is expected to provide insights into the tunable color emission of metal-coordinated supramolecular bimetallic gels, facilitating an understanding of their fine-tuning capabilities.

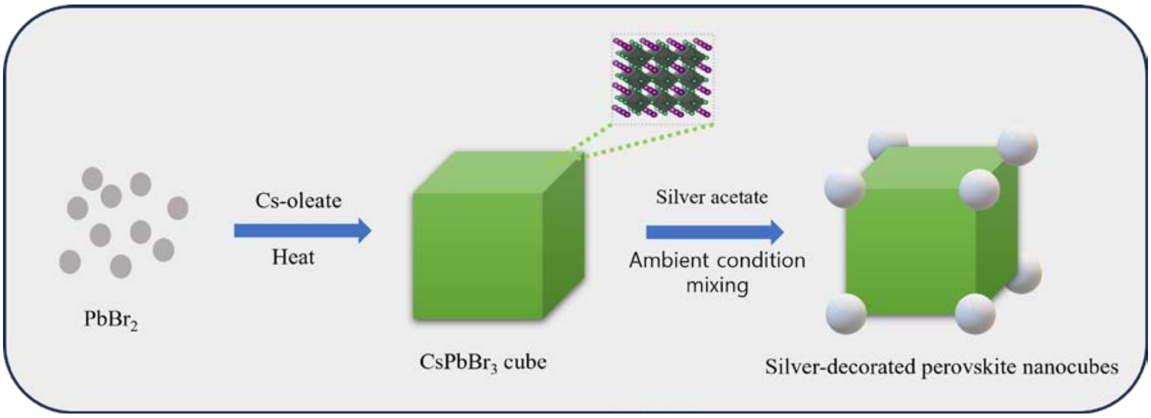
Poster Presentation : **INOR.P-105**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Plasmonic Augmentation of Photoluminescence in CsPbBr3 Perovskite Nanocubes via Silver Nanoparticles Attachment at Ambient Conditions

Levan Ratinai, **Kwangyeol Lee**[1,*]

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

In recent years, perovskites have attracted worldwide attention as light-emitting materials for next-generation quantum dot LEDs (QLEDs). All-inorganic perovskites are attracting increasing attention due to their unique stability, and in-depth research on their composition and structure for high photoluminescence quantum yield (PLQY) and high stability is ongoing. Herein, we present a novel method to produce silver/lead halide perovskite heterostructures in the ambient condition to achieve desired optoelectrical characteristics utilizing exciton/plasmon interactions. The study's outcomes hint at broad implications for advancing photonic and optoelectronic devices, highlighting ambient-temperature nanoparticle attachment as a promising avenue for material enhancement. The succinct integration of plasmonic nanoparticles and perovskite structures opens new pathways for the development of efficient optoelectronic applications, from light-emitting devices to solar cells and photodetectors, signifying a leap forward in harnessing the synergistic potential of hybrid material systems.


PbBr$_2$
Cs-oleate
Heat
CsPbBr$_3$ cube
Silver acetate
Ambient condition mixing
Silver-decorated perovskite nanocubes

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Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Modulation of the Proton Conduction Behavior with Atomic Precision in Covalent Organic Frameworks

Gyuhyeong Lee, Chang Seop Hong[1,*], Eunsung Lee[*]

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

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

In recent years, proton conductivity studies in covalent organic frameworks (COFs) have emerged as promising strategies for the development of advanced materials that can be used for energy conversion and storage. Especially, stable π-π stacking layered structure of two-dimensional (2D) COFs facilitates proton transfer through aligned channels. The highly tunable structure can significantly influence the physicochemical properties of COFs, thereby enhancing the efficiency of proton conduction within COFs. The rational design and synthesis of crystalline COFs offer a valuable approach to gaining insights into the underlying mechanisms of proton conduction. Herein, we report the synthesis and characterization of pyridine-based COFs (PyPA-FPA, PyPA-FNA). Pyridine moieties are a key to proton conductivity through hydrogen bond interaction with protons. Interestingly, variations in the position of nitrogen atoms within pyridine-based COFs result in distinct proton conduction behaviors. Phosphoric acid (PA) as a proton source is successfully loaded into COFs and proton conductivity (σ) of PA@PyPA-FNA can reach 4.55×10^{-2} S cm^{-1} (353 K, 90% RH). A change in conductivity according to the nitrogen position of pyridine is expected, and DFT calculation was performed to confirm the correlation.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Controlling supramolecular copolymerization of alkynylplatinum(II) terpyridine complexes: from isodesmic to cooperative mechanisms

Sehee Kim, Sung Ho Jung*, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

Recently, cooperative supramolecular polymerization has garnered considerable attention due to its significant potential for enabling controlled chain-growth polymerization, which offers a route to achieving a well-defined degree of polymerization and low polydispersity. In this study, we synthesized two distinct alkynylplatinum(II) complexes, one bearing a saturated long alkyl chain (Pt-Sat-C18) and another containing a diacetylene moiety within a long alkyl chain (Pt-DA-C25). Spectroscopic analyses revealed that Pt-Sat-C18 undergoes supramolecular polymerization via an isodesmic pathway, while Pt-DA-C25 assembles cooperatively. Intriguingly, the mechanism of supramolecular copolymerization could be tuned by varying the composition ratios: transitioning from an isodesmic to a cooperative pathway was achieved by increasing the proportion of Pt-DA-C25. Moreover, UV irradiation prompted a shift from an isodesmic to a cooperative assembly mechanism. Morphologically, self-assembled Pt-Sat-C18 resulted in left-handed fibrillar structures, whereas Pt-DA-C25 led to left-handed tubular assemblies. Supramolecular co-assembly further revealed helical ribbon or tubular structures. Photoluminescent properties were also observed, with emission spectra centered at approximately 650 nm, attributed to the formation of excimer species facilitated by strong Pt···Pt interactions. To elucidate the mechanisms underlying these supramolecular polymerizations, temperature-dependent UV-visible spectroscopy was conducted during the cooling /heating processes, and thermodynamic parameters for both isodesmic and cooperative pathways were quantitatively assessed through curve fitting.

Poster Presentation : **INOR.P-108**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

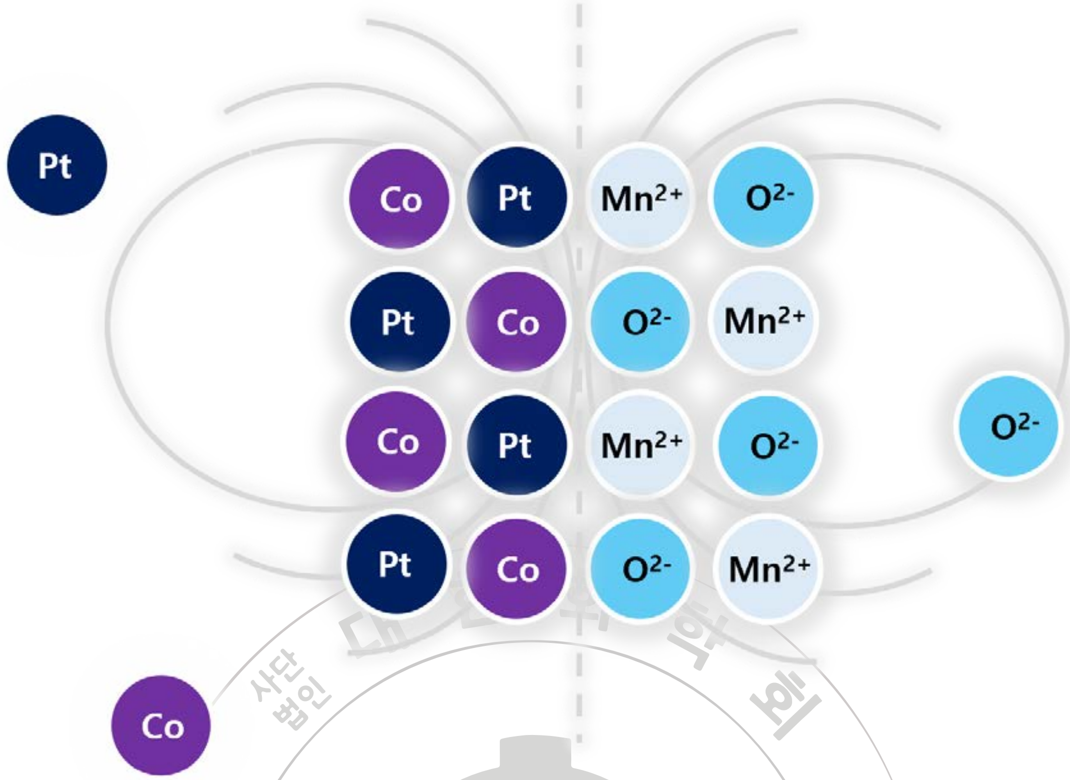
Trace the atomic migration in the intermetallic phase transformation with the $Pt_3Co@MnO$ core-shell interface interaction

<u>Jeong Yujin</u>, Kwangyeol Lee[1,*]

The department of chemistry, Korea University, Korea

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

Controlling the crystal structure of Pt–M (M = transition metal) nanoalloys to chemically ordered ones has drawn increasing attention in oxygen reduction reaction (ORR) electrocatalysis due to their high resistance against M etching in acid electrolytes. Although Pt-Co alloy nanoparticles (NPs) have demonstrated respectable initial ORR activity in acid, their stability remains a big challenge due to the fast etching of transition metals. In this work, The ordered Mn-doped Pt_3Co NPs are synthesized for the first time by employing a core/shell $Pt_3Co@MnO$, MnO shell could provide abundant O-vacancies for facilitated Pt/Co atom diffusion and prevent NP sintering during thermal annealing. Interestingly, The MnO shell facilitated intermetallic phase transformation at lower temperatures. This phenomenon creates an electrostatic electric field of atoms at the core-shell interface, and this electric field rearranges the surrounding atoms, propagating the intermetallic phase, making conversion to the intermetallic phase possible.


Pt
Co
Pt
Mn^{2+}
O^{2-}
Pt
Co
O^{2-}
Mn^{2+}
Co
Pt
Mn^{2+}
O^{2-}
O^{2-}
Pt
Co
O^{2-}
Mn^{2+}
Co

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Poster Presentation : **INOR.P-109**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

IZCp and PZCp: Redox Non-innocent Cyclopentadienyl Ligands as Electron Reservoirs for Sandwich Complexes

Seunghyuk Yoo

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

A long-sustained effort of systematic steric and electronic modification of cyclopentadienyl (Cp) ligands has enabled them to find wide-ranging valuable applications. Herein, we present two novel Cp ligands: imidazolium- and pyrrolinium-substituted zwitterionic Cps (IZCp and PZCp), whose key utility is redox non-innocence – ability to participate cooperatively with the metal center in redox reactions. Through the simple metalation of ZCps, the Cr(0) and Mo(0) half-sandwich complexes ($Cr(IZCp)(CO)_3$, $Cr(PZCp)(CO)_3$, $Mo(IZCp)(CO)_3$ and $Mo(PZCp)(CO)_3$) respectively, as well as the Ru(II) sandwich complexes ($[Ru(IZCp)(Cp)]PF_6$ and $[Ru(PZCp)(Cp)]PF_6$) were prepared. The sandwich complexes were fully characterized and showed by cyclic voltammetry reversible one-electron reduction at $E_{1/2}$ potentials ranging from −1.7 to −2.7 V vs. Fc/Fc^+. These values are unusually low and have not been observed with other Cp ligands due to the instability of the reduced complexes. DFT calculations for the reduced derivatives with IZCp and PZCp (Cr(0) and Mo(0) half-sandwich complexes, Ru(II) sandwich complexes) showed their spin densities to be highly delocalized over their ZCp ligand moieties (70%–90%). EPR analysis of the isolated $K[Mo(PZCp)(CO)_3]$ and Ru(PZCp)(Cp) also indicated a high degree of ligand-localized radical character. Thus, the IZCp and PZCp ligands act as electron reservoirs to sustain these Mo and Ru complexes in highly reduced states. At the same time, the CO stretching frequencies of $K[Mo(PZCp)(CO)_3]$: νCO 1871, 1748, and 1699 cm^{-1}, rank the $[PZCp]^-$ ligand as the strongest electron-donating Cp ligand among the re-ported $CpMo(CO)_3$ derivatives, whose νCO > 1746 cm^{-1}. In addition, these redox non-innocent Cps were obtained in high yields and found to be practically air- and moisture-stable, unlike typical Cps.

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Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Solvent-Driven Dynamics: Crafting Tailored Transformations of Cu(II)-Based MOFs

Cheol Yeong Heo, Nak Cheon Jeong[*]

Department of Physics & Chemistry, DGIST, Korea

Metal–organic frameworks (MOFs), a sort of crystalline porous coordination polymers composed of metal ions and organic linkers, have been intensively studied for their ability to take up nonpolar gas-phase molecules such as ethane and ethylene. In this context, interpenetrated MOFs, where multiple framework nets are entwined, have been considered promising materials for capturing nonpolar molecules due to their relatively higher stability and smaller micropores. This study explores a solvent-assisted reversible strategy to interpenetrate and deinterpenetrate a Cu(II)-based MOF, namely, MOF-143 (noninterpenetrated form) and MOF-14 (doubly interpenetrated forms). Interpenetration was achieved using protic solvents with small molecular sizes such as water, methanol, and ethanol, while deinterpenetration was accomplished with a Lewis-basic solvent, pyridine. Additionally, this study investigates the adsorptive separation of ethane and ethylene, which is a significant application in the chemical industry. The results showed that interpenetrated MOF-14 exhibited higher ethane and ethylene uptakes compared to the noninterpenetrated MOF-143 due to narrower micropores. Furthermore, we demonstrate that pristine MOF-14 displayed higher ethane selectivity than transformed MOF-14 from MOF-143 by identifying the “fraction of micropore volume” as a key factor influencing ethane uptake. These findings highlight the potential of controlled transformations between interpenetrated and noninterpenetrated MOFs, anticipating that larger MOF crystals with narrower micropores and higher crystallinity will be more suitable for selective gas capture and separation applications.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Revealing Dynamic Weak Coordination Bonding of Halocarbons and Its Role for Activation of Metal-Organic Frameworks.

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Daegu Gyeongbuk Institute of Science & Technology, Korea

[1]*Department of Physics & Chemistry, DGIST, Korea*

Coordination bonds play a crucial role in numerous inorganic chemical reactions. Strong coordination bonds have been extensively studied because they are easily observable with conventional instruments. However, characterizing weak coordination bonds poses challenges due to technical limitations. In this poster, we present the weak coordination bonding ability of halocarbons with lone pair electrons on neutral halogen atoms using a metal-organic framework (MOF) as a platform. By utilizing Cu3(BTC)2 featuring a distinctive Cu-Cu stretching vibrational band, we estimated the coordination strength of a confined neutral halogen atom binding to an axial Cu(II) site through Raman spectroscopy. Furthermore, we demonstrated the tendency in coordination strength based on the period of the halogen atom, the number of halogen atoms in the molecule, and the functional group. We proved the weak coordination ability for chemical activation purposes. As a result, halocarbon molecules exhibited the capacity to coordinatively exchange all previously confined solvent molecules within the pores. It was confirmed that Cu3(BTC)2 could be fully activated even when placed in a vacuum at room temperature, underscoring the weak coordination strength in this process.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Hydrolytic Stability Enhancement of HKUST-1 by introducing polymers through catalytic polymerization

Inhoo Kim, Nak Cheon Jeong*

Department of Physics & Chemistry, DGIST, Korea

Metal-organic frameworks (MOFs) are relatively novel materials composed of inorganic metal ions and organic linkers. These systems have shown potential as porous materials in different applications such as chemical separation, gas sorption, catalysis, chemical sensing, and electric conductivity due to their chemical tunability, offering different physicochemical properties and structural functionalities.A prominent feature in MOFs is that the inorganic fragment of the framework can possess open-metal sites (OMSs), which are vacant Lewis sites on the metal ions. These sites have been demonstrated to play critical roles in relevant applications, and thereby, distinct methodologies have been developed to access these sites. However, despite their potential in various applications, fundamental studies of the interaction between OMS and guest molecules are still insufficient. Meanwhile, a particular challenge for MOFs with OMS is the fragility of the framework to external factors such as moisture or acidic environment that collapse the material. In this work, we have focused on studying the molecular interaction between OMSs and guest molecules in confined spaces based on the characteristics of MOFs and methods to enhance the hydrolytic stability of MOFs. We hypothesized that introducing polymers inside the nano space to increase the hydrolytic stability of water-susceptible MOFs would prevent the structure from distorting, thus preventing phase change or collapse. On the other hand, since the already synthesized long-chain polymers cannot physically enter the small pores of MOFs, we aimed to introduce polymers through catalytic polymerization by using coordination bonding between monomers and OMSs. We selected HKUST-1, which consists of copper ions and benzene tricarboxylate (BTC) ligands, and it is well known for its low hydrolytic stability. As the starting monomer, we chose anisidine as a good candidate for catalytic polymerization because it can coordinate at the OMSs of HKUST-1 and its polymerization is initiated by heat in the presence of a copper catalyst.After introducing the polymers in the pores of the copper paddle wheel-based MOF, substantial enhancement of the hydrolytic stability of HKUST-1 was observed, to the extent that its structure remained intact even after exposure to humid air for one year.

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Poster Presentation : **INOR.P-113**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Mole-Ratio Effects on the Formation of Supramolecular Complexes of a Linear Dipyridyl Ligand

Kyu Won Lee, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

Synthesis of a linear dipyridyl ligand (L) incorporating an O_2S_2-crown ether and its mole-ratio-dependent coordination modes in the formations of silver(I) complexes are reported. The reaction of L with $AgClO_4$ afforded a loop-type 1D coordination polymer $[Ag_2(L)(ClO_4)_2]_n$ (1). In the mole-ratio variation experiments, notably, the use of 3.0 equiv or above the amount of $AgClO_4$ in the same reaction condition gave a double-stranded 1D coordination polymer 2, $[Ag_3(L)(ClO_4)_3]_n$. To monitor the observed mole ratio-dependent endo-coordination products as well as their reactivities, systematic powder X-ray diffraction (PXRD) analysis has also been applied.

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Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

pseudo[1]Catenane-Type Pillar[5]arene Derivatives Exhibiting Chiral Inversion by External Stimuli

Hankyeol Park, Eunji Lee[1,*]

Department of chemistry, Gangneung-Wonju National University, Korea

[1] *Department of Chemistry, Gangneung-Wonju National University, Korea*

Pillar[n]arene derivatives have planar chirality due to two enantiomers (*pS* and *pR*) by rotation of the aromatic unit around the methylene bridges. A pillar[n]arene-based bicyclic pseudocatenane was constructed to realize chiral inversion of the pillar[n]arene core by external stimuli, including pH, redox, solvents, and temperature. In this presentation, we report the chiral inversion of a single molecule induced by metal ions or guest molecules. *pseudo*[1]catenane-type pillar[5]arenes (L^1 and L^2) containing crown ethers with different donor atoms were synthesized and the two enantiomers (*in*-*pS*-form and *in*-*pR*-form) were isolated by chiral column chromatography. The circular dichroism (CD) spectrum demonstrated that chiral inversion occurred only when mercury ions were added. Furthermore, chiral inversion occurred by the conformational transformation in the presence of an excess of dinitrile guest molecule.

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Poster Presentation : **INOR.P-115**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis and Structural Characterization of Metallosupramolecules Based on a Benzyl Mercaptan-Attached Pillar[5]arene

Jaejun Lee, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

We proposed a flexible linear ligand characterized by the free rotation of the ethylene group between donor atoms, leading to structural diversity in their respective complexes. In this work, a pillar[5]arene incorporating a benzyl mercaptan subunit to induce pi interactions was synthesized and its metallosupramolecules are reported. L was synthesized by the reaction of pillar[5]-dibromide and benzyl mercaptan in the presence of sodium metal. Metallosupramolecules with soft metal ions were prepared and its crystal structures were characterized.

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Pillar[5]arene-based 2D Ag(I) Coordination Polymer Showing Dimensional Change by Guest Molecules

Seohyeon Yun, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

The thiobenzonitrile-attached pillar[5]arene derivative (L) was synthesized to examine the guest-induced interlocked system. The reaction of L with $AgClO_4$ afforded a two-dimensional (2D) coordination polymer $[Ag(L)(ClO_4)]_n$ (1) which has a diagonal herringbone-type 2D sheet. In the presence of the 1,2-dicyanoethane (C2) guest and 1,5-dicyanopentane (C5) guest molecules, a 1D poly-*pseudo*[1]catenane, $[Ag(C2@L)(ClO_4)]_n$ (2) and $[Ag_2\ (C5@L)(ClO_4)_2]_n$ (3) was also obtained, respectively. The guest molecules thread into the pillar[5]arene cavity and the sulfur atoms on both arms and the cyano groups of guests coordinate with the silver(I) ions to form a *pseudo*[1]catenane. Furthermore, the cyano group of the adjacent ligand binds to the silver(I) atom, forming a 1D chain. Furthermore, the reaction of L with $AgClO_4$ in the presence of 1,8-dicyanooctane (C8) guest gave a 1D poly-*pseudo*[1]catenane $[Ag_2\ (C8@L)(ClO_4)_2]_n$ (4) which have different coordination mode.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

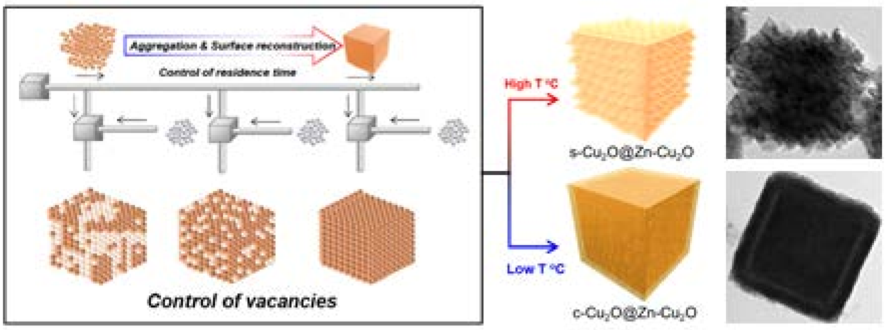
Synthesis of spiky Cu_2O@Zn-doped-Cu_2O selective for C_{2+} products in CO_2 electroreduction by controlling vacant site of Cu_2O via flow

Heeju Moon, Kwangyeol Lee[1,*]

chemistry, Korea University, Korea

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

Herein, we developed spiky/cubic core-shell Cu_2O@Zn-doped-Cu_2O nanoparticles (NPs) as catalysts for selectively converting CO_2 to multi-carbon (C_{2+}) products such as ethylene and ethanol. C_{2+} products have been evaluated as desirable compounds due to their high energy densities. We could quantify the amount of Zn doping in NPs by adjusting the surface vacancies and reconstruction degree using a microfluidic reactor. Moreover, we found that the post-incubation temperature determined the morphologies, spiky or cubic shapes, of Cu_2O@Zn-doped-Cu_2O NPs. Consequently, we demonstrated that the spiky Cu_2O@Zn-doped-Cu_2O NPs have more remarkable selectivity for C_{2+} products.



Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Improved Ethylene Selectivity in CO_2 Reduction Reaction by Introducing Ag Core within Cu_3N Nanoparticles.

MinSeon Cha, Kwangyeol Lee[1,*]

Korea University, Korea

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

Achieving carbon neutrality has become a significant global concern since the late 20th century, with increasing public interest over the years. One effective approach to reaching carbon neutrality is the transformation of CO_2 into useful chemicals like CO, ethanol, and ethylene. The conversion of CO_2, a simple one-carbon molecule, into ethylene, a more complex two-carbon molecule featuring a double bond, is a challenging yet highly sought-after process due to ethylene's substantial market value, estimated at 230 billion US dollars in 2021. Copper (Cu) is recognized for its effectiveness in carbon-carbon coupling during CO_2 reduction reactions. The combined forms of Cu(0) and Cu(I) in Cu_3N nanocrystals enhance the stability and ethylene selectivity of the catalyst during electroreduction. Our research presents the creation of an Ag@Cu_3N nanocatalyst through seed-mediated growth designed for CO_2 electroreduction. Incorporating an Ag core is key to generating *CO, an essential intermediate in carbon-carbon coupling. This Ag@Cu_3N nanocatalyst exhibits high selectivity for ethylene at low potentials, aligning with industrial requirements for the CO_2 reduction reaction.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Studies on Inter- and Intra- Molecular Interactions in Circular Dimeric Metal Complexes

Jiyeong Song, Young-A Lee*

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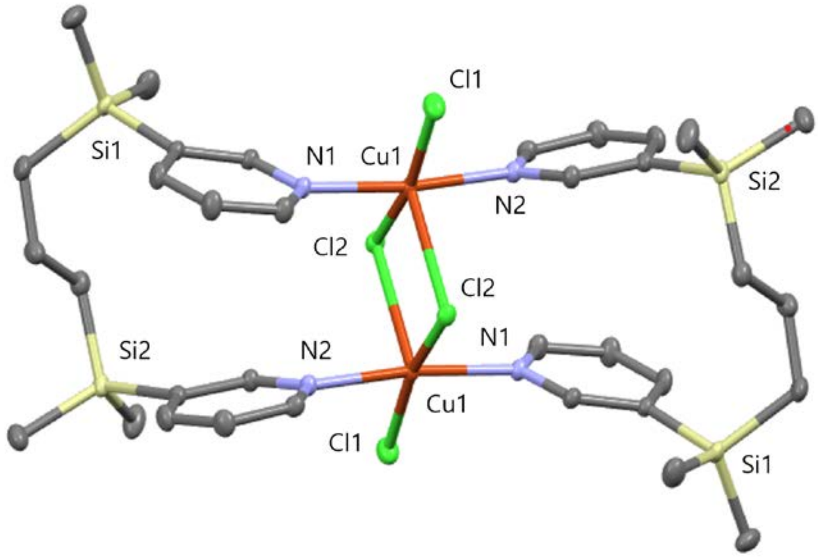
Single crystals were obtained through the self-assembly of various metal salts and a bidentate ligand (L) (L = 1,3-bis(dimethyl(pyridin-3-yl)silyl)propane)) at room temperature, and their physical properties were studied. In this case, complexes have formed a circular dimeric structure where a nitrogen atom is coordinated to metal ions. For the $[CuL]Cl_2$ complex, the distance between Cu(1) and both nitrogen atoms was 2.01(2) Å, and the bond angle (N(1)-Cu(1)-N(2)) is 171.99°. There is an Cu(1)···Cu(1) intra-interaction (Cu(1)···Cu(1)#1 = 3.45(8) Å) but no interaction between other Cu metal ions. For another case, $[ZnL]I_2$, the distance is too long to have intra-interaction (Zn(1)···Zn(1)#1 = 8.14(4) Å) and any interactions between inter-Zn metal ions. In this study, we examined the characteristics of these circular dimeric metal complexes, which are influenced by the size and properties of the metal. And we investigated the effects of various anions and solvents.


Cl1
Si1
N1
Cu1
N2
Si2
Cl2
Cl2
Si2
N2
N1
Cu1
Cl1
Si1

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Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

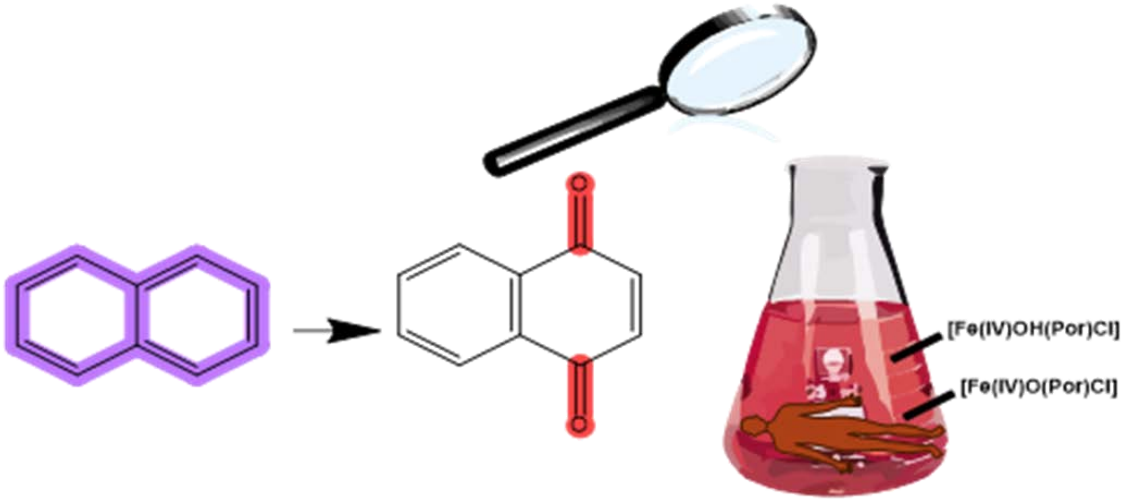
The Mysteries of Aromatic Oxidation: A DFT investigation into [Fe(IV)OHPor(Cl)] Complex's Reaction Mechanism.

Steiny Russelisaac Premakumari, **Kyung-Bin Cho**[1,*]

Chemistry, Jeonbuk National University, Korea

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

Developing organometallic catalysts that are green, efficient and stable for the selective direct oxidation of aromatic C-H bonds under mild conditions is a challenging task due to their high stability. Despite this challenge, scientists worldwide are making persistent efforts to improve both catalytic activity and selectivity. We focus on a series of structurally diverse metalloporphyrin compounds, with particular attention given to the high-valent iron and manganese complex. These complex serves as a key oxidative intermediate in heme and non-heme enzymes, which catalyze essential biochemical processes[1]1. The study investigates the direct hydroxylation of aromatic C-H bond using the active catalyst [Fe(IV)OH(Por)Cl]. Through theoretical analysis, the study uncovers the reaction mechanism for the simple aromatic hydroxylation of naphthalene to naphthalene-1,4-diol and its subsequent oxidation to naphthalene-1,4-dione. The investigation reveals that both oxygen atom transfer (OAT) and hydrogen atom transfer (HAT) mechanisms are involved in the studied process.s[2]2 Moreover, a contracting reactivity pattern is observed during the investigation, where the FeIVOH species is more reactive than the FeIVO species. The study also examines the relative oxidative abilities of these two species in a congruent reaction. These findings provide valuable insights into the mechanism of the oxidation reaction and demonstrate the potential of [Fe(IV)OH(Por)Cl] as a catalyst for the efficient production of naphthalene-1,4-dione.Keywords: C-H activation; aromatic hydroxylation; organometallic catalyst; OAT; References1.K.-B. Cho, X. Wu, Y.-M. Lee, Y. H. Kwon, S. Shaik and W. Nam, Journal of the American Chemical Society, 2012, 134, 20222-20225.2.S. Bang, Y.-M. Lee, S. Hong, K.-B. Cho, Y. Nishida, M. S. Seo, R. Sarangi, S. Fukuzumi and W. Nam, Nature Chemistry, 2014, 6, 934-940.


[Fe(IV)OH(Por)Cl]
[Fe(IV)O(Por)Cl]

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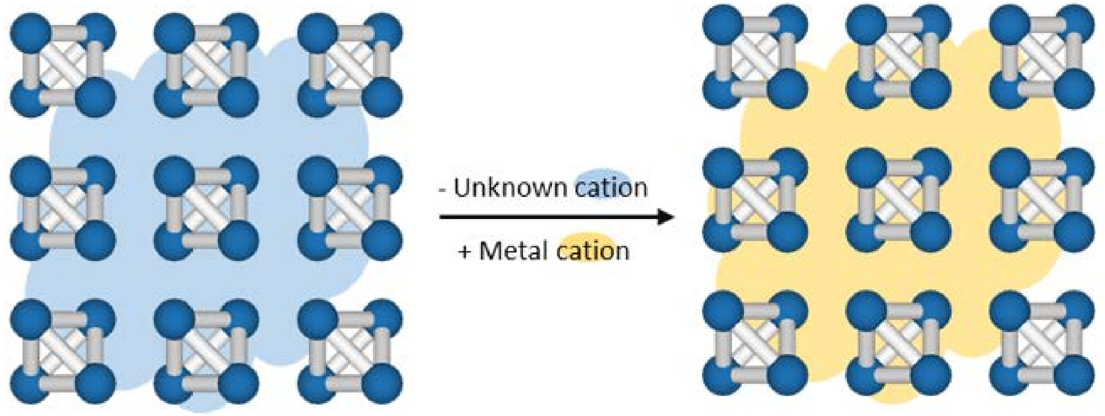
Poster Presentation : **INOR.P-121**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Controlling Cationic Species inside Zr-Based Metal-Organic Polyhedra

Eunjie Ju, Wonyoung Choe[1,*]

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

Metal-organic polyhedra (MOPs), a member of metal-organic materials (MOMs), are cage-based compounds, composed of metal clusters and organic linkers. Among them, Zr-based MOPs are becoming an emerging class of porous materials due to their remarkable chemical and mechanical stability. In previous works, we reported cation exchange strategy for residual cationic species in Zr-based MOPs (UMOP-1). Here, we demonstrate metal cation exchange strategy that controls residual cationic species in UMOP-1. To our surprise, the lithium cation exchanged UMOP-1 shows superprotonic conductivity (≥ 10-2 Scm-1). We expect the Zr-based MOPs as promising platform for proton conductors.



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Poster Presentation : **INOR.P-122**

Inorganic Chemistry

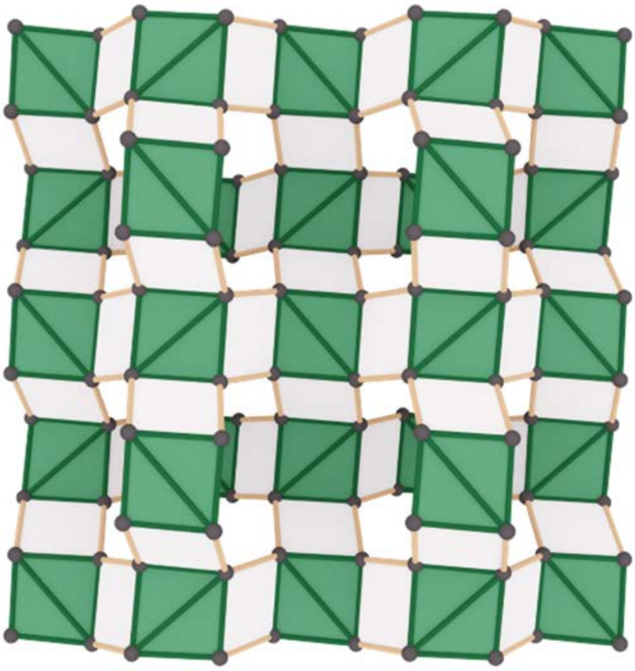
Exhibition Hall 2 FRI 11:00~13:00

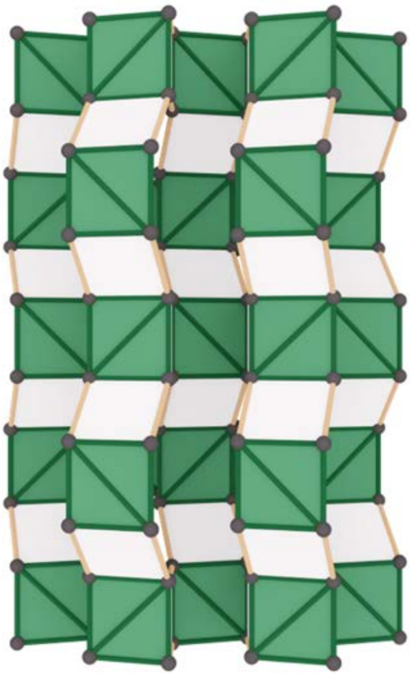
Pressure and Guest-Responsive Zeolitic Imidazolate Framework as Solid-State Molecular Kirigami

Joohan Nam, Eunji Jin[1], Leila Abylgazina[1], Jürgen Getzschmann[1], Wenlong Xue[2], HongKyu Lee, Hyunchul Oh, Hoi Ri Moon[3], Sebastian Henke[2], Andreas Schneemann[1,*], Wonyoung Choe[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Inorganic Chemistry I, Technische Universität Dresden, Germany*
[2]*Anorganische Chemie, Technische Universität Dortmund, Germany*
[3]*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*

Paper craft, including origami and kirigami, has become a cross-cutting theme from art to industry. Kirigami-inspired design principles allow to establish three-dimensional mechanical linkages with unprecedented mechanical properties. Herein, we report a zeolitic imidazolate framework (ZIF) displaying folding mechanics based on kirigami tessellation. Pressure and guest-induced responses demonstrated the kirigami mechanism of the ZIF, wherein imidazolate linkers act as hinges. This discovery of the concealed kirigami tessellation inside a flexible ZIF reveals foldable mechanics at the molecular level.





Poster Presentation : **INOR.P-123**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

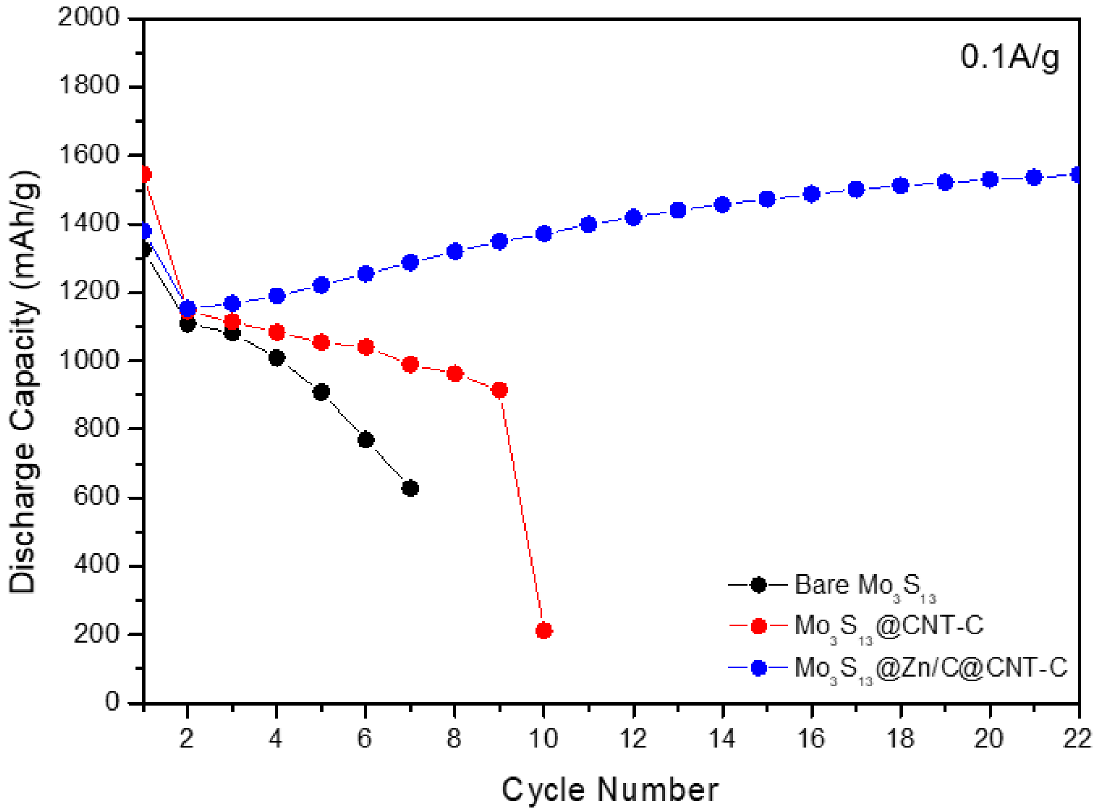
Facile synthesis of Mo_3S_{13} cluster and composite with MOF-derived carbon as anode material for Li-ion Batteries

Hosung Hwang, Cho Se Youn[1,*]

Carbon composite materials research center, Korea Institute of Science and Technology, Korea

[1] *Carbon Convergence Materials Research Center, Korea Institute of Science and Technology, Korea*

Lithium-ion batteries (LIBs) have been widely used as energy storage devices, particularly for mobile devices and electric vehicles. So far, graphite is a mainstream material as an anode due to its high stability and electro-conductivity. However, its potential for improving energy density is limited due to its low theoretical capacity (374 mAh g^{-1}), Therefore, there is a need to develop new anode materials with a high specific capacity. Transition metal chalcogenides are one of the promising candidates because of their high theoretical capacity. Specifically, molybdenum sulfide species (MoS_2, MoS_3, Mo_3S_{13} cluster, MoS_x) are well known as conversion-type electrodes with extraordinary potential for electro-performance in LIBs. Moreover, wide interlayer spacing of molybdenum sulfides increases the diffusion coefficient of Li+ and prevents structural collapse during lithiation/delithiation. Among these molybdenum sulfide species, Mo_3S_{13} cluster is expected to possess the highest capacity owing to its high content of the sulfur configuration. Despite these advantages, Mo_3S_{13} cluster have barely been studied as materials for LIBs because of complex and long preparation steps (7 days), low electro-conductivity, and poor cycle stability. In this work, we prepared Mo_3S_{13} clusters with a facile synthesis method (1 day) and composited the Mo_3S_{13} clusters with a carbon source from a MOF-derived carbon for increasing electro-conductivity and preventing volume expansion. In addition, the MOF-derived carbon prevents aggregation of the Mo_3S_{13} cluster, thereby increasing reaction sites with Li+ ions and resulting in a capacity increase.


0.1A/g
Discharge Capacity (mAh/g)
0
200
400
600
800
1000
1200
1400
1600
1800
2000
Cycle Number
2
4
6
8
10
12
14
16
18
20
22
Bare Mo_3S_{13}
Mo_3S_{13}@CNT-C
Mo_3S_{13}@Zn/C@CNT-C

Poster Presentation : **INOR.P-124**
Inorganic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Density Functional Theory Study: Transition Metal Ion catalyzed Tyrosine activation and Di-tyrosine Cross-linking with Reactive-Oxygen Species

Youngseob Lee, Kyung-Bin Cho[1,*]

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

Amyloid fibrils that are considered to be the cause of Alzheimer's disease(AD) are highly stable and insoluble amyloid plaques in the neuropil. Redox-active metal ions such as Cu^{2+}, and Fe^{3+} have been suggested to play a key role in many neurodegenerative disorders including Alzheimer's disease(1). Metal-protein interactions could result in oxidative stress through generation of reactive oxygen species(ROS) such as H_2O_2. In 2013 Al-Hilaly *et al.* investigated the formation of di-tyrosine cross-links in the amyloid-β (42) peptide by covalent coupling of two tyrosine residues, which has been implied to play a key role in the development of the Alzheimer's disease(2). In this point of view, using density functional theory we studied about tyrosine radical formation and di-tyrosine cross-linking catalyzed by several transition metal ions such as Fe(II), Cu(II), Cu(I), Co(II) and Ni(II) with H_2O_2 as the ROS in B3LYP/Def2-TZVPP level.

Reference

1) Bush et al, Curtain CC: Twenty years of metallo-neurobiology: where to now? Eur Biophys J 2008, 37:241-245
2) Al-Hilaly et al. A central role for dityrosine crosslinking of Amyloid-β in Alzheimer's disease, Acta Neuropath. Commun. 2013, 1, 83.

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Poster Presentation : **INOR.P-125**

Inorganic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

How to Selectively Control the Four Structures of Lanthanum-based MOFs.

Su Jeong Sim, Woo Ram Lee[1,*]

Hallym University, Korea

[1] *Department of Chemistry and Institute of Applied Chemistry, Hallym University, Korea*

Synthesizing MOFs (Metal-Organic Frameworks) involved the use of lanthanide metal nitrate and H3TPO (tris(4-carboxyphenyl)phosphine oxide). It was observed that depending on solvothermal reaction conditions like the acidity, temperature, and the kind of lanthanide metal ion utilized, the coordination number of the metal ions, the structure of SBUs (Secondary Building Units), cell parameters, and the charge of frameworks varied. Synthesized MOFs were classified based on their structures, and trends and synthesis mechanisms were analyzed to comprehend how alterations in synthesis conditions influence structures of MOFs.

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Poster Presentation : **PHYS.P-55**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Photochemistry of Thymine in Solution and DNA Revealed by an Electrostatic Embedding QM/MM Combined with Mixed-Reference Spin-Flip TDDFT

Maryam Farmani, **Cheol Ho Choi**[1,*]

Chemistry, Kyungpook National University, Iran

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

The photochemistry of nucleobases, important for their role as building blocks of DNA, is largely affected by the electrostatic environment in which they are soaked. For example, despite the numerous studies of thymine in solution and DNA, there is still a debate on the photochemical deactivation pathways after UV absorption. Many theoretical models are oversimplified due to the lack of computationally accurate and efficient electronic structure methodologies that capture excited state electron correlation effects when nucleobases are embedded in large electrostatic media. Here, we combine mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT) with electrostatic embedding QM/MM using electrostatic potential fitting fitted (ESPF) atomic charges, as a strategy to accurately and efficiently describe the electronic structure of chromophores polarized by an electrostatic medium. In particular, we develop analytic expressions for the energy and gradient of MRSF/MM based on the ESPF coupling using atom-centered grids and total charge conservation. We apply this methodology to the study of solvation effects on thymine photochemistry in water and thymine dimers in DNA. In the former, the combination of trajectory surface hopping (TSH) nonadiabatic molecular dynamics (NAMD) with MRSF/MM remarkably revealed accelerated deactivation decay pathways, which is consistent with the experimental decay time of ～400 fs. The enhanced hopping rate can be explained by the preferential stabilization of corresponding conical interactions due to their increased dipole moments. Structurally, it is a consequence of characteristic methyl puckered geometries near the conical intersection region. For the thymine dimer in B-DNA, we found new photochemical

pathways through conical intersections that could explain the formation of cyclobutadiene dimers and 6−4 photoproducts.

Poster Presentation : **PHYS.P-56**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Molecular Aggregation Behavior and Microscopic Heterogeneity in Binary Osmolyte-Water Solutions

Jiwon Seo, Ravi Singh, Jonghyuk Ryu, Jun-Ho Choi*

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

Osmolytes are small organic compounds that modulate the stability and solubility of protein in aqueous solutions. Tetramethylurea (TMU), urea, acting as destabilizing osmolytes, and a protecting osmolyte, trimethylamine-N-oxide (TMAO), and dimethyl sulfoxide, known as a cryoprotectant, are fully miscible with water under ambient conditions, but they exhibit different aggregation behavior in microscopic level. We performed MD simulation with graph theoretical analysis and calculated *h*-value, which quantitatively measures the spatial inhomogeneity of given molecules, in various binary osmolyte-water solutions to understand microscopic heterogeneity and operating mechanism of osmolyte molecules. TMAO, acting as a protecting osmolyte, does not exhibit a noticeable self-aggregation behavior even at 10 m, while forming preferential interaction with water. On the other hand, a destabilizing osmolyte, TMU, tends to from self-associated aggregates via hydrophobic interaction and they avoid interaction with water. The increase in self-association between osmolyte molecules results micro-heterogeneous distribution of osmolyte and water molecules with high h-value. Taken together, it is suggested that both hypotheses of direct mechanism, focus on the direct interaction between osmolytes and proteins, and indirect mechanism, emphasizing the modulation of water H-bond network by osmolytes, are involved in the mode of osmolyte action.

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Poster Presentation : **PHYS.P-57**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Quantitative analysis of the Li-ion solvation structure using ATR-FTIR spectroscopy

Taewoo Kim, Kyungwon Kwak[*], Minhaeng Cho[*]

Department of Chemistry, Korea University, Korea

Attenuated total reflection–Fourier transform infrared (ATR-FTIR) spectroscopy is employed to study condensed materi-als owing to the convenience of sample preparation and measurement, as well as its ability to prevent signal saturation. Recently, it has been applied to in-situ and in-operando observations of chemical reactions inside electrochemical devic-es like lithium-ion batteries. However, as ATR-FTIR spectroscopy generates spectra based on reflectance, quantitative measurements of chemical species using the Beer–Lambert law is challenging. Despite the availability of several correc-tion methods to address these issues, discrepancies exist between the solvation structure around Li+ ions obtained by transmission-type FTIR and ATR-FTIR spectroscopies, complicating quantitative analysis. Here, we investigated ATR correction algorithms, explored the reasons for discrepancies between ATR-FTIR and transmission-type FTIR spectros-copy results, and developed a method to align the results, and solvation structure around Li+ ion. These findings are cru-cial for enhancing the accuracy of experiments conducted using ATR-FTIR spectroscopy.

Poster Presentation : **PHYS.P-58**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

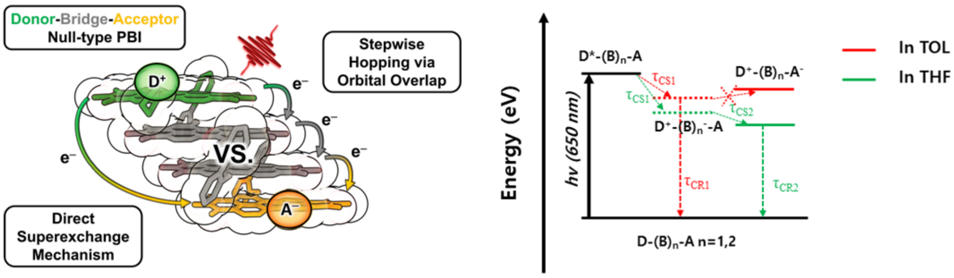
Exponential Distance Dependence of Photoinitiated Stepwise Electron Transfer in Null-Type Coupling PBI Arrays

Dongho Kim*, **Würthner Frank**[1,*], **Leander Ernst**[1], **Hongwei Song**

Department of Chemistry, Yonsei University, Korea

[1]*Institut fu̍r Organische Chemie & Center for Nanosystems Chemistry, Wu̍rzburg Universita̍t, Germany*

Recently, the unconventional slip-stacked aggregates with null-type coupling have received considerable attention due to their unique photophysical properties, which can be controlled by the intra- or inter-molecular π–π stacking geometries. The compensation of short-range charge-transfer (CT) mediated (orbital overlap) and long-range Coulomb (dipole-dipole interaction) coupling in PBI arrays leads to a vanishing overall coupling, prevents excimer state formation and results in different excited-state dynamics. In our study, we have combined steady-state measurements, spectroelectrochemistry and femtosecond transient absorption spectroscopy to investigate the photophysical process within the null-type coupling PBIs array. Here in trimer and tetramer we provide definitive experimental evidence that the electron transfer to PBI acceptor in polar solvent occurs with the coupling of two mechanisms: coherent superexchange with attenuation factor β = 0.2 Å -1 (the lower limit of superexchange regime) and incoherent stepwise charge hopping mechanism. In polar solvent, it seems that the energy level of final charge separation state (D+-B-A-) is more sensitive than that of intermediate charge separation state (D+-B--A) and this stabilization of final charge separation state induces large driving force for superexchange electron transfer from donor to acceptor. The detailed distance and solvent polarity dependence study of the null-type coupling PBIs array with electron donating and withdrawing group substitution constitutes an important fundamental step toward the understanding of competitive photophysical processes in the context of controlled molecular geometries and brings greater possibility for their application to artificial photosynthesis.


Donor-Bridge-Acceptor
Null-type PBI
Stepwise Hopping via Orbital Overlap
D+
A−
e−
e−
e−
e−
VS.
Direct Superexchange Mechanism
Energy (eV)
hv (650 nm)
D*-(B)n-A
D+-(B)n-A-
D+-(B)n--A
τCS1
τCS1
τCS2
τCR1
τCR2
D-(B)n-A n=1,2
In TOL
In THF

Poster Presentation : **PHYS.P-59**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Investigation of Protein-Peptide Binding Using Artificial Intelligence and Large-Scale Molecular Dynamics

Se-Jun Kim, Hyungjun Kim, Jeong-Mo Choi[1,*]

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

Various biological phenomena within living organisms mainly rely on the interactions of biomolecules. Among these interactions, protein-peptide binding emerges as one of the pivotal mechanisms in processes such as cellular signaling. To comprehend this binding behavior, structural simulations, most notably molecular dynamics simulations, can be employed to identify and analyze conformational changes, binding sites, and binding affinities. These simulations can provide structural information at the atomistic scale, and various methods have been developed to calculate thermodynamic quantities from simulation trajectories. However, challenges arise when dealing with proteins and peptides whose structures have not been experimentally determined, as the experimental structures are required for structure-based simulations. To unveil the structures and binding characteristics of protein-peptide complexes, we propose a novel approach that integrates AlphaFold2 with large-scale molecular dynamics simulations. The emergence of AlphaFold2, an artificial intelligence model, has enabled the prediction of relatively accurate protein structures. This breakthrough expands the feasible structural space for calculations. Our analysis commences with a residue-wise examination to unravel the molecular principles underlying the formation of protein-peptide complexes. Furthermore, we employ umbrella sampling to compute the theoretical binding affinity, explaining the mutational effect on the binding. We believe that our protocol can be used not only to understand the binding process but also to identify key residues and structural motifs crucial for these interactions.

Poster Presentation : **PHYS.P-60**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Impact of cationic lipid composition and tail conformation on thermodynamic properties of lipid bilayers

Sungjun Lim, Hyonseok Hwang[*]

Department of Chemistry, Kangwon National University, Korea

Cationic lipids dare key components in mRNA vaccines, which have recently gained significant research interest as drug delivery vehicles. For the mRNA (drug) to enter cells, it must undergo endocytosis, where cationic lipids, capable of effectively binding to the negatively charged cell membranes, play an important role. In this work, we performed molecular dynamics (MD) simulations to investigate the impact of the composition of cationic lipids on lipid bilayers using two types of lipids: DOTAP (1,2-dioleoyl-3trimethylammonium-propane), a cationic lipid, and DOPC (1,2-dioleoyl-sn-glycero-3-phosphocholine), a zwitterionic lipid. Generally, both lipids have cis double bonds at the carbons 9 and 10 of tails, However, simulations were also conducted by modifying the lipid tails to trans double bonds for a comparison of the characteristics between systems with cis and trans double bonds. Thermodynamic properties such as area per lipid, bilayer thickness and tail order parameter were calculated with respect to the different fraction of DOTAP and tail conformation. Several issues associated with the charged head group and tail conformation of lipids are also addressed in this study.

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Poster Presentation : **PHYS.P-61**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Exploration of conformational structure of 2-butanone by IR resonant VUV-PI/MATI mass spectroscopy

Sung Man Park, Chan Ho Kwon*

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

2-Butanone (C_4H_8O), emitted by plants, fungi, and bacteria, influences the composition and chemistry of the atmosphere by introducing free radicals into the upper troposphere. Spectroscopic studies, including IR and Raman spectroscopy, have suggested the presence of two conformers in 2-butanone at room temperature: trans and gauche conformers. Understanding the structures and physicochemical properties of these conformers is crucial for comprehending the related chemical reactions in atmospheric chemistry. Here, we investigated the conformational structures of 2-butanone using IR resonant vacuum ultraviolet (VUV) photoionization (PI)/mass-analyzed threshold ionization (MATI) mass spectroscopy. Under cold conditions of a molecular beam of 2-butanone, comparison of IR resonant VUV-PI and IR dip VUV-MATI spectra confirmed a single conformer population. Quantum chemical calculations predicted that this conformer has the trans conformation. In addition, constructing the multidimensional potential energy surface associated with the conformational interconversion revealed that the trans conformer is more stable than the gauche conformer by ~600 cm^{-1}, with a low energy barrier of ~10 cm^{-1} from gauche to trans. It suggests that the conformational population depends on molecular beam conditions. Subsequent experiments under various molecular beam conditions are planned to acquire information about the gauche conformer.

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Poster Presentation : **PHYS.P-62**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Valence Orbitals Ordering and Cationic Structure Depending on Fluorine Substitutions at the *Ortho* Position of Pyridine Using VUV-MATI Mass Spectroscopy

Hyojung Kim, Sung Man Park, Chan Ho Kwon[*]

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Korea

Halopyridines, where hydrogen atoms in pyridine are substituted with halogen atoms, have garnered considerable attention from physical chemists due to the significant impact of the position and number of substituted halogen atoms on the energy ordering of valence molecular orbitals. In a previous study on 2-fluoropyridine (2-FP), it was discovered that the stability of nonbonding orbitals increases owing to the interaction between the lone-pair sp^2 orbital of nitrogen in pyridine ring and the nonbonding orbital of the adjacent fluorine atom. This interaction led to a reversal in the energy ordering of the two outermost valence orbitals (σ and π orbitals) of pyridine. Subsequently, to delve deeper into the influence of the number of substituted fluorine atoms on the energy ordering of valence orbitals in pyridine, 2,6-difluoropyridine (2,6-DFP) was investigated. In 2,6-DFP, two fluorine atoms are substituted at each ortho position adjacent to the lone-pair sp^2 orbital of nitrogen. This investigation utilized vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) mass spectroscopy and compared the findings with those of 2-FP. Key insights were deduced by examining the ionization-induced geometric changes, corroborated by the Franck-Condon simulations. The results suggest that the energy ordering of the two outermost valence orbitals in 2,6-DFP closely resembles that of 2-FP. However, the stability of nonbonding orbitals in 2,6-DFP increased, resulting in a higher excited electronic state (D_1) of the 2,6-DFP cation compared to that of 2-FP cation.

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Poster Presentation : **PHYS.P-63**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Isomer- and conformer-specific vibrational spectroscopy of 3-penten-1-yne by IR resonant VUV-MATI mass spectroscopy

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Propene (CH_2CHCH_3) and ethynyl radical (C_2H) are chemical species of interest in astrochemistry, discovered in the Taurus Molecular Cloud and Titan, and have been the subject of various spectroscopic and dynamical studies. In this study, we explored the neutral and cationic states of trans- and cis-3-penten-1-yne, proposed as a product of the reaction between propene and ethynyl radical, using IR resonant vacuum ultraviolet (VUV) photoionization (PI)/mass-analyzed threshold ionization (MATI) mass spectroscopy. The 3-penten-1-yne sample, containing both trans and cis isomers, was synthesized, and the VUV-MATI spectrum was measured. The adiabatic ionization energy of the 3-penten-1-yne was determined using the origin band of the measured VUV-MATI spectrum, resulting in 9.0499 ± 0.0006 eV. Quantum chemical calculations of two isomers in 3-penten-1-yne were utilized to elucidate the cationic vibrational structure from the VUV-MATI spectrum and obtain information about the neutral vibrational structure from the IR resonant VUV-PI spectrum. The vibrational assignment of each isomer could be accomplished and furthermore, the composition of the two isomers in the 3-penten-1-yne sample was determined, which was compared with NMR data. The synthetic routes dominantly producing each isomer in the 3-penten-1-yne sample were developed, and their IR resonant VUV-PI/MATI spectra are compared with those of the 3-penten-1-yne sample.

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Poster Presentation : **PHYS.P-64**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Investigating charge recombination dynamics in blue-TiO2 composites revealed by transient absorption spectroscopy

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Titanium dioxide (TiO2) is an inorganic semiconductor photocatalyst and has been used for the various photocatalytic applications due to its excellent catalytic activity and superb chemical stability. To improve the photocatalytic activity of TiO2, blue TiO2, called as B-TiO2, was suggested and was readily prepared from the direct reduction of pristine TiO2. B-TiO2 including the high density of oxygen defect showed the enhanced photocatalytic activity originating from the panchromatic absorption of sunlight. In this study, we aimed to investigate the underlying excited-state dynamics in B-TiO2 by comparing with that in the pristine TiO2. To do so, we implemented the nanosecond transient absorption spectroscopic (ns-TA) experiments based on the real-time tracking manner. Especially, we employed the various chemical conditions such as the uses of electron and hole scavenger in order to study the effect of the environmental condition in the photo-induced electronic dynamics.

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Physical Chemistry
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Structural perturbation from protein-dye interaction revealed by X-ray solution scattering

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Fluorescent dyes have been widely used for cell imaging and bio-molecular analysis in the fields of molecular biology and biochemistry due to its emitting property and binding affinity to the biomolecules. The detailed information about the interaction between protein and dye in terms of protein conformation is elusive. In this study, we aim to reveal the structural interaction on the protein-dye complexes by using the combination of optical spectroscopies and X-ray solution scattering. As a target system, we prepared the hemoglobin (Hb)-dye complexes by using various organic dyes under the physiological condition. The binding constants (Ka) and ratio (n) of the dye-protein complexes were determined from the systematic spectroscopic measurements. Based on those results, we focused on the structural characterization using small/wide-angle X-ray solution scattering (SAXS/WAXS). The molecular structures of protein-dye complexes were directly extracted from the experimental scattering curves with the aid of newly-developed structural analysis based on the molecular dynamics (MD) simulation.

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Physical Chemistry
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Revealing the photochemistry of CdS/S-g-C3N4 heterojunction interface during the CO2 reduction by using time-resolved laser spectroscopy

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Graphitic carbon nitride (g-C3N4) has been attracted as a metal-free photocatalyst in order to generate the solar chemicals via the direct reduction reaction from CO2. Recently, we developed the heterojunction architecture consisted of sulfur-doped g-C3N4 and CdS composite, named as CdS/S-g-C3N4 heterojunction composite. This compound showed the generation of HCOOH from CO2 with an excellent efficiency. Based on the developed photocatalytic system, we performed the transient absorption and time-resolved photoluminescence spectroscopic experiments for the reaction phase. From this way, it was revealed that the presence of the interfacial heterojunction in CdS/S-g-C3N4 showed the expression of the long-lived charge separated state, linked to the enhancement of photocatalytic efficiency. The systematic spectroscopic measurements combined to the structural characterization of as-synthesized material provide the photochemical insights for the photo-induced charge carrier dynamics in the CdS/S-g-C3N4 heterojunction composite.

Poster Presentation : **PHYS.P-67**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Delayed fluorescence from inverted singlet and triplet excited states of heptazine analogues HzT-FEX2 by Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT)

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In this study, we investigate the photophysical properties of heptazine analogues, specifically HzT-FEX2, using Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT). Heptazine derivatives are promising candidates for applications in optoelectronics and photovoltaics due to their remarkable stability and electronic properties. Understanding the mechanisms behind their delayed fluorescence is crucial for optimizing their performance in these applications. Our study focuses on the inverted singlet and triplet excited states (i.e., T1

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Physical Chemistry

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Role of small charged biomolecules under liquid-liquid phase separation of FUS Protein

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The formation of protein aggregates, particularly involving the FUS (FUsed in Sarcoma) protein, has been identified as a major factor contributing to the development of amyotrophic lateral sclerosis (ALS). The FUS protein, with a net positive charge of +14 e, comprises a negatively charged (-4 e) low complexity domain (LCD) known for its intrinsically disordered region, and a positively charged (+18 e) C-terminal domain (CTD) under physiological conditions. This study aims to elucidate how small charged biomolecules influence the liquid-liquid phase separation (LLPS) of the FUS protein through charge-charge interactions, employing fluorescence microscopy. Given the positively charged and negatively charged ends of the full-length FUS protein, it exhibits a spontaneous self-assembling tendency. Consequently, the LLPS pattern remained largely unchanged when either ATP or spermine was introduced. However, LLPS was observed at the negatively charged N-terminus upon the addition of spermine, while the positively charged C-terminus responded to ATP addition. Intriguingly, the full-length FUS protein displayed increased LLPS in cells when both ATP and spermine were present. This suggests that small charged biomolecules such as ATP and spermine can induce or enhance the LLPS of charged proteins within cells.

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Physical Chemistry
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Machine Learning-Enhanced Quantitative Analysis of CWA chromogenic detection

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This study introduces a machine-learning augmented quantitative analysis of chromogenic reaction outcome between chemical warfare agents and detection papers with chromogenic chemosensors (M8, M9). Aforementioned detection papers are designed to detect liquid phase chemical warfare agents (drops, aerosol), the presence of which manifests developing characteristic and visible coloring. Focusing on G-series nerve agents, specifically GB (Sarin) and GD (Soman), we attempted interpreting the outcomes (color changes), which triggered by chromogenic reaction, with the help of machine-learning process. Controlled amount, but varying concentrations of GB and GD are applied to the detection papers and resultant color after 24 hours, when wet papers and color changes no more develop, were documented. A controlled photographic setup was employed to ensure consistent shooting condition and to acquire objective data set. The colorimetric changes were then analyzed using a machine learning model, aiming to overcome the limitations of subjective human interpretation and enhance the quantitative assessment of the detection papers.This research contributes to the field of chemical safety by providing a more accessible and efficient detection method, emphasizing the importance of integrating machine learning into traditional detection techniques. The study also lays a foundation for future research in expanding the detection range and enhancing algorithmic accuracy in diverse environmental conditions.

Poster Presentation : **PHYS.P-70**

Physical Chemistry

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Analyzing Chemical Warfare Agents (CWAs) Decontamination Rates of Rotorcrafts Through Flight: A Combined Experimental and Computational Study

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Given the persistent threat posed by Chemical Warfare Agents (CWAs) in both military and civilian spheres, our research aims to address critical gaps in understanding the dynamics of CWA decontamination on rotorcraft surfaces. This study employs a novel approach by integrating comprehensive experimental protocols with advanced computational simulations to provide a comprehensive understanding of the decontamination process.Methodologically, we adopted a dual-pronged strategy. Experimentally, we conducted tests replicating real-world flight conditions to observe CWA behavior, with a specific emphasis on the persistence of VX on aircraft surfaces. Computationally, Density Functional Theory (DFT) was utilized to model the molecular interactions between CWAs and aircraft materials, offering profound insights into underlying chemical processes.Our research findings emphasize the significant resilience of CWAs, notably VX, a highly toxic nerve agent, and its strong affinity for aluminum surfaces, thus complicating decontamination efforts. These results were corroborated by our computational models, which underscored the potential for accelerated material degradation stemming from oxidation reactions facilitated by CWA exposure.This study underscores the urgent necessity for the development of advanced decontamination methodologies capable of effectively mitigating the persistence of CWAs like VX on rotorcraft surfaces. The insights garnered from our interdisciplinary analysis not only enhance our comprehension of CWA dynamics but also provide a

foundation for future research endeavors aimed at devising more robust defense strategies against chemical threats, thus significantly contributing to both military readiness and civilian safety protocols.

Poster Presentation : **PHYS.P-71**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Screening inhibitors against SOD1(A4V) using computational calculations

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The copper-zinc superoxide dismutase (SOD1) is the protein which associates with amyotrophic lateral sclerosis (ALS). SOD1 mutation at codon 4 from alanine to valine (A4V) is one of the most aggressive forms of ALS. SOD1(A4V) is a cause of the aggregation in SOD1 that often affects muscle weakness in initial symptoms and respiratory failure in the last stage of symptoms. Although there is one available drug to target for SOD1 mutation, that drug has side effects on patients. Therefore, this study aims to screen the chemicals to be the novel inhibitors for targeting SOD1(A4V). In this study, 15 pharmacologically active compounds were studied, in terms of inhibiting SOD1 aggregation, using molecular docking and quantum calculations. The results showed that Idarubicin of 15 compounds showed the best binding affinity (-8.3 kcal/mol) with SOD1(A4V) due to strong hydrogen bonding interaction hydrogen bond interactions with Arg115 of SOD1(A4V).

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Physical Chemistry

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Polyamines and Metal Ions on Amyloid Beta(1-42) Protein Aggregation

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Amyloid beta is implicated in the development of Alzheimer's disease, but the underlying mechanisms remain unclear. In this study, we investigated the influence of positively charged substances, including polyamines and metal ions, on the aggregation of amyloid beta protein. Results revealed that amyloid beta aggregated into condensates and fibrils under various conditions. Initially, the quantities of condensates and fibrils varied depending on the incubation time. A shorter incubation time resulted in a higher observation of condensates, while an increase in incubation time led to a decrease in the quantity of condensates and an increase in the quantity of fibrils. Secondly, the quantities of condensates and fibrils varied depending on the concentration of spermine, a type of polyamine. It was observed that as the concentration of spermine increased, the quantity of fibrils decreased, while the quantity of condensates increased. Furthermore, the positively charged magnesium ions also exhibited a trend where an increase in their concentration led to a decrease in the quantity of fibrils and an increase in the quantity of condensates.

Poster Presentation : **PHYS.P-73**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Structural and optical properties of nitrogen-implanted ALD-grown ZnO films

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ZnO naturally exhibits an n-type structure due to stoichiometric inconsistencies during the growth process, and can easily grow n-type semiconductors by doping group III elements such as Al. Ga, In. However, p-type ZnO is known to be difficult to grow due to dopants and compensation effects, and p-type ZnO has been reported through doping elements such as N, NH3, As, Sb, and P and co-doping N and Ga. It has been intended to fabricate stable p-type ZnO material through advanced particle beam injection technology and to conduct research to identify the p-type ZnO through space- and time-resolved quantum spectroscopic analysis. In this study, we fabricated the N-doped ZnO films by nitrogen implantation on the atomic layer deposition (ALD)-grown ZnO films at different post-annealing temperature, and then analysed cross-sectional image and crystallographic information of the N-doped ZnO films by electron microscopy, focused ion beam, and X-ray diffraction. Spectroscopic study was also performed by the UV-Vis reflectance, steady-state photoluminescence (PL), and time-resolved PL to elucidate internal photophysics of excited charged carrier dynamics.

Poster Presentation : **PHYS.P-74**

Physical Chemistry

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The Influence of Bismuth Electrode Hydrophilic Properties on the Selectivity of Electrochemical Carbon Dioxide Reduction Products

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The impact of surface hydrophilicity on the electrocatalytic behavior of bismuth electrodes during CO_2 reduction in aqueous conditions was explored in this study. Two distinct bismuth film types, namely Bi/Cu and Bi/eCu/Ti, were fabricated and evaluated for their electrocatalytic performance within a reduction potential range of -0.776 to -1.376 V vs RHE. The Bi/Cu film surfaces exhibited a composition of granular particles (400 – 800 nm), while the Bi/eCu/Ti films displayed nanoscale roughness, incorporating smaller nanostructures (a few tens of nanometers) alongside granular particles.In the reduction process, both CO_2 and H_2O molecules competed for reaction on the surfaces of both bismuth film types, resulting in formate and H_2 as the primary products of reductive reactions, respectively. Interestingly, under identical conditions, the Bi/eCu/Ti configuration demonstrated both lower and higher selectivities for formate and H_2 compared to the corresponding Bi/Cu cases, despite having similar bismuth film thicknesses. This variation was attributed to the enhanced hydrophilicity of the Bi/eCu/Ti bismuth film surfaces, stemming from surface nanoscale roughness and lower surface carbon contents when compared to the Bi/Cu surfaces.The findings of this study propose a novel strategy for controlling product selectivity in electrocatalytic CO_2 reduction under aqueous electrolytes through surface engineering. Specifically, the deliberate manipulation of bismuth film surface characteristics, such as nanoscale roughness and hydrophilicity, offers a promising avenue for tailoring the outcome of CO_2 reduction reactions

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Physical Chemistry
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Exciton Dynamics in a Molecular Aggregate using Pump-Probe Spectroscopy

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We aim to understand and control the photoinduced dynamics of a variety of systems spanning from simple model molecules to complex materials composed of multiple constitu-ents. We are interested in the investigation of molecular aggregates using ultrafast time-resolved spectroscopy. Molecular aggregates provide how exciton in materials would ideally behave in the event of photoexcitation because we can now better connect the structure-property relationships. To understand the exciton transport in a molecular aggregate made of perylene bisimide (PBI-OR), we plan to control the degree of aggregation of PBI-OR under various solvent conditions. Aggregation of PBI-OR may lead to the formation of excimers and charge trans-fer upon photoexcitation. When aggregation is controlled by varying the polarity from a non-polar solvent to a polar solvent, exciton transport in different PBI-OR aggregates can be systematically quantified and understood using transient absorption spectroscopy with a range of pump fluence and energy. Additionally, we will analyze the structures of PBI-OR aggregates from various solvents by using transmission electron microscopy (TEM).

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Poster Presentation : **PHYS.P-76**
Physical Chemistry
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Enhancing accuracy of absorption spectroscopic measurements in saturated absorbers

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In absorption spectroscopy, quantum fluctuations within the intensity of an optical probe act as a noise that limits measurement accuracy. Increasing the intensity of the optical probe holds the potential to improve measurement precision, yet high probe power often brings the issue of reduced accuracy due to sample saturation. This study systematically analyzes the accuracy of absorption measurements by selecting an appropriate absorption model, with a particular focus on evaluating the impact of sample saturation under both classical and quantum probe conditions. The primary goal of our research is to determine the optimized probe intensity. To this end, we observed changes in measurement accuracy corresponding to varying intensities of probes in Coherent state, Fock state, and Squeezed state. This research aims to reveal critical characteristics of the absorption model when varying the parameters such as saturation probe light intensity, excited-state lifetime, and absorption cross-section. Absorption spectroscopy is an essential tool in various fields, including chemistry, biology, and environmental science, where exceeding specific probe intensities for samples can often result in irreversible damage. Therefore, we expect this study can contribute to finding the optimal probe intensity that aligns with the characteristics of the sample in absorption spectroscopy. The findings of this research will aid in maximizing measurement accuracy and minimizing the risk of sample damage in various applications utilizing absorption spectroscopy.

Poster Presentation : **PHYS.P-77**

Physical Chemistry

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Non-Adiabatic Semi-Classical Dynamics Study of The Bidirectional PCET Process of NH_3Cl

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We recently reported the quantum wave-packet propagation (QWP) study of the bi-directional proton-coupled electron transfer (PCET) process starting from the charge-transferred (CT) excited state ($H_2N^+HCl^-$) of NH_3Cl with three diabatic potential energy surfaces (PESs) in reduced three-dimensional (3D) space based on reactant Jacobi coordinates. The study has shown that the proton transfer (PT) process (producing H_2N and HCl) dominates over the electron transfer (ET) process (generating H_2NH and Cl). The extension of the QWP study to full dimensional space (9D), however, is not straightforward. In the present work, we carried out the nonadiabatic dynamics starting from the $H_2N^+HCl^-$ in full dimensional (9D) space using the Surface-Hopping including ARbitary Couplings (SHARC) with the CASPT2 level of ab initio theory (SHARC/CASPT2). The proper active space for the SHARC/CASPT2 calculations was investigated by comparing the energetic data of NH_3Cl derivatives given from the CASPT2 with various active spaces as well as the results of Weizmann–2 (W2) theory. Then, the statistical changes of nuclear motions, PESs, population dynamics, and branching ratio were investigated from the ensemble of classical trajectories. More detailed microscopic insights into the PCET process of $H_2N^+HCl^-$ will be discussed based on the present results in full dimensional space.

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Physical Chemistry
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Mind the Gap: Energy Gap for Protein Binding

Chan-Gyu Kim, TaeHwan Kim, Jeong-Mo Choi*

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Statistical mechanics of protein folding can be explained by the gap theory, which suggests that there must be an energy gap between the native state and the lowest-energy non-native state in order to correctly describe the behaviors of natural proteins, such as first-order-like transition of folding. Inspired by the gap theory, the μ-potential has been developed to semi-quantitatively describe protein folding. The μ-potential is a statistical scoring function that assigns a negative energy score to native contacts and a positive energy score to non-native contacts, and it has been used to distinguish between native and decoy protein structures. In this study, we expand the application of the μ-potential to protein binding, as the positive and negative design principle is also intrinsic in a protein-protein interaction. This implies that the energy gap between the native complex structure and non-native structures is also required for successful protein binding.

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Physical Chemistry
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Conformation-Selective Ultraviolet Photofragmentation Spectra of Ubiquitin Ions in a Cryogenic Ion Trap

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Obtaining ultraviolet photo-fragmentation (UVPF) spectra of protein ions in the gas phase has been challenging due to their low fragmentation yields. Here, we introduce a novel approach to acquire UVPF and conformation-selective UV-UV hole burning (HB) spectra of multiply charged ubiquitin ions ((Ubi+zH)+z, z=7-10) generated via electrospray ionization. Our approach involves generating (Ubi+zH)+z(N2)m ions within a cryogenic ion trap by binding multiple N2 molecules to the ions. Upon exposure to a UV laser pulse, efficient fragmentation of (Ubi+zH)+z(N2)m ions occurs, yielding primarily bare (Ubi+zH)+z ions as fragments. The substantial mass difference between the parent ((Ubi+zH)+z(N2)m) and fragment ions ((Ubi+zH)+z) facilitates the acquisition of UVPF or UV-UV HB spectra by distinguishing the fragment ions generated by UV pump and probe pulses. The UV-UV HB spectra revealed the presence of at least two distinct conformers. Molecular dynamics simulations indicate that these conformers represent the A-state structures, differing only in the interactions of a tyrosine residue with neighboring residues. This study demonstrates that UV-UV HB spectroscopy of protein ions bound with multiple N2 molecules provides a potent tool for investigating diverse structural isomers of protein ions.

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Physical Chemistry

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Charge Underscreening of Lithium Ion-Doped Ionic Liquids: Across Short-range to Long-range Structures

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Due to nonvolatility, nonflammability, and high thermal stability, Li^+ doped ionic liquids have been considered as next-generation electrolytes for energy storage devices. Li^+ ion is not only a charge carrier but also affects the structure of surrounding anions and the overall viscosity. Meanwhile, the effect of Li^+ doping on the charge screening is not yet well understood despite their close relation to the electric double layers, activity coefficients, and differential capacitance. Especially, in these concentrated electrolytes, unexpectedly long-range screening was reported, which is contrary to what is expected from the Debye-Hückel theory and remains unanswered. Thus, we investigate the relation between the structures and the charge screening in Li^+ doped ionic liquids. We conduct atomistic molecular dynamics simulations for 1-butyl-1-methylpyrrolidinium bis(trifluoromethyl sulfonyl)imide ([Pyr14][TFSI]) with varying Li[TFSI] fractions ($f_{Li[TFSI]}$=0, 0.1, 0.2 and 0.3) and find that the screening length decreases with $f_{Li[TFSI]}$. We analyze pair correlation functions and find that Li^+ ions mainly distort the short-range structures of anions. In addition, we estimate charge density fluctuation from local charge densities and show that charge density fluctuation increases with $f_{Li[TFSI]}$. We conclude from our simulations that Li^+ ions induce the short-range distortion of ion structures, which facilitates charge density fluctuations. These enhanced charge density fluctuations could act as effective charges in solvents and might lead to diminished screening length in Li^+ doped ionic liquids.

Poster Presentation : **PHYS.P-81**

Physical Chemistry

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Molecular Dynamics Simulation Analysis of FOX Transcription Factors Interacting with DNA in the Context of Environmental Toxicology

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Abstract: Gene expression, a pivotal process for cellular function, is intricately regulated by transcription factors that bind specific DNA sequences to modulate gene activity. Among these, Histone H1 is renowned for its critical role in sustaining DNA structure within nucleosomes during gene expression. Notably, Forkhead Box A1 (FOXA1), a FOX protein family member, has been discovered to substitute Histone H1 functions, altering DNA conformation and offering fresh perspectives on gene regulation. Our study delves into these novel findings with a focus on environmental toxicology. Through computational simulations, we analyzed various DNA-protein complexes and mutations, including FOXA1-DNA interactions. These simulations assessed key parameters such as Root-Mean-Square Deviation (RMSD) and Root-Mean-Square Fluctuation (RMSF), DNA-protein contact points, and DNA bending. Crucially, we expanded our investigation to include the potential impact of environmental toxins on these interactions. By doing so, we aim to elucidate how contaminants might perturb FOXA1's role in gene regulation, which could have profound implications for cellular homeostasis and organismal health in contaminated environments.

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Exploring Jacob’s Ladder: Density Sensitivity in Density-Corrected Density Functional Theory

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Density functional theory (DFT) is a quantum computational method that balances computational cost and accuracy, finding widespread utility across numerous fields today. However, the DFT has a density-driven error, which is an error that occurs when the DFT produces the wrong density. Density-Corrected Density Functional Theory (DC-DFT) uses a density other than the density that produced self-consistently to resolve this error. One practical example of this approach is HF-DFT, which employs the Hartree-Fock (HF) density. Pinpointing these density-driven errors necessitates access to the exact density, a task complicated by the numerical intricacies involved in Kohn-Sham (KS) inversion. Density sensitivity emerges as a critical metric, gauging the extent to which changes in density influence both the energy computations of the system and the employed functionals. Density sensitivity can be used to determine the potential for reducing density-driven errors by applying HF-DFT. Density sensitivity may vary depending on the functionals used, but there is limited knowledge about it. The purpose of this study is to investigate the relationship between density sensitivity and several properties depending on the functional rung.

Poster Presentation : **PHYS.P-83**

Physical Chemistry

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SERS Activity of Electromagnetic and Charge Transfer Effects on PS/Ag/MoO_3 Film by RF Magnetron Sputtering

Yoonseop Byun, Shuang Guo, Young Mee Jung*

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In this study, a radio frequency (RF) magnetron sputtering system was used to fabricate PS/Ag/MoO_3 films. The films were fabricated by depositing layers Ag and MoO_3 on a polystyrene substrate. Our study focuses on the electromagnetic (EM) effect and charge transfer (CT) in semiconductor as a function of film thickness. Thickness variations were achieved by changing the sputtering time for Ag. The metal-semiconductor molecular interface was investigated by studying surface-enhanced Raman scattering (SERS) spectra using 4-mercaptobenzoic acid (4-MBA) as a probe molecule. The findings contribute to the research and development of semiconductor-based SERS substrates through the exploration of EM and CT effects. This has the potential to pave the way for customized applications in the field of SERS. The details of the results will be discussed in this presentation.

Poster Presentation : **PHYS.P-84**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Study on the effect of vitamins on cellular expression level of MMP-2

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Matrix metalloproteinase-2 (MMP-2) belongs to the Zinc-metalloenzymes family and plays crucial roles in various physiological and pathological processes. Under normal conditions, MMP-2 participates in tissue remodeling, wound healing, and angiogenesis by degrading components of the extracellular matrix. Its primary function involves the degradation of type IV collagen within the extracellular matrix (ECM). However, MMP-2 also tightly involves the progression of cancers, where elevated levels within tumor cells facilitate cancer advancement and metastasis. In addition, many diseases such as cervical cancer, Alzheimer’s disease, stroke, cardiovascular diseases are related to the expression level and activity of MMP-2. Targeting of MMP-2 has emerged as a promising strategy in cancer therapy Vitamins have been considered to be the effective anticancer agents by inhibiting MMP’s expression and activity. Here, we investigated the effect of different vitamins' treatment on MMP-2 expression, examined on Hela cell. Our findings revealed that vitamin A and D effectively inhibited MMP-2 expression, whereas other vitamins such as C, B3, and E showed no discernible effects. Interestingly, when vitamins C, B3, and E were combined with vitamins A and D, they not only failed to inhibit MMP-2 expression but also diminished the effectiveness of vitamins A and D in downregulating MMP-2 expression.

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Poster Presentation : **PHYS.P-85**

Physical Chemistry

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Study of hyaluronic acid-based hydrogels for drug delivery

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Hydrogels have been extensively investigated as a model for tissue engineering, drug delivery and control release because of their properties such as softness, high-water-controllable swollen and biocompatibility. Among hydrogels, photo-responsive hydrogel which has been a great interest, has opened a new approach for studying on drug delivery. Here, we synthesized light-controllable hydrogels using maleimide-modified hyaluronic acid and photo-dissociable dimeric Dronpa(pdDronpa) which is photo-switchable green fluorescent protein. The hydrogels underwent reversible gel-sol transition due to photo-dissociation and re-association of pdDronpa upon cyan and violet light, respectively. In addition, we synthesized insulin-containing hydrogels by inserting Alexa594-conjugated insulin molecules into the hydrogels and observed that insulin was released by cyan light illumination. Furthermore, released amount of insulin could be controlled by illumination time.

Poster Presentation : **PHYS.P-86**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

De novo nanobody binder design by generative AI models

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This study focuses on an innovative approach within the field of protein engineering, aiming to discover novel nanobody candidates with enhanced binding affinity to Green Fluorescent Protein (GFP). We used RFdiffusion, a generative AI, to design the CDR loop backbone structure. The ProteinMPNN model was applied to generate optimized amino acid sequences for the designed backbone structure. The CDR structure and amino acid sequence were integrated through Rosetta fix-backbone design, forming a complete protein structure. The resulting protein structure was refined using Rosetta relaxation. To assess designed nanobody structure quality, we predicted GFP binding strength indirectly using Rosetta score. We identified nanobody candidates predicted to exhibit higher binding affinities with GFP than conventional ones. Chosen candidates will undergo experimental validation to confirm their efficacy. This study introduces a novel pipeline by incorporating Generative AI into conventional protein engineering research, enabling the rapid and effective design of new proteins. Furthermore, it is expected to contribute to the discovery of novel nanobody binder with real-world applications.

Poster Presentation : **PHYS.P-87**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Photodissociation Dynamics of Nitroaryl caged DEA-NONOate probed by Time-resolved IR Spectroscopy

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In this study, we investigated the photochemical dynamics of Nitroaryl-DEA NONOate, which holds promising potential for photoresponsive selective NO release. This compound can release nitric oxide (NO) at low concentrations, inducing vasodilation, and at high concentrations, triggering apoptosis in cancer cells.Initially, femtosecond laser-driven time-resolved IR spectroscopy (TRIR) was employed to study the dynamics of Nitroaryl-DEA NONOate excited by 400 nm photons, designed to induce π-π* transitions of the nitroaryl group. Combining quantum chemical calculations and molecular dynamics simulations, we predicted the photochemical reaction mechanism.The results of this study were compared with the photochemical dynamics of molecules with similar structural motifs, such as V-PYRRO/NO. The research aims to compare and analyze the NO release mechanisms depending on the wavelength and explore new application possibilities by investigating the reaction under lower energy conditions.

Poster Presentation : **PHYS.P-88**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Predicting Chemical Compound Solubility with GPT Models: A Comparative Analysis

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This study investigates the use of GPT-4.0 for in-context learning and fine-tuned GPT Turbo 3.5 to predict the log solubility of chemical compounds, showcasing the adaptability of language models to the field of chemistry. By employing in-context learning with GPT-4.0 and fine-tuning techniques on GPT Turbo 3.5, we evaluated their efficacy in predicting chemical properties. The fine-tuned GPT-3.5 model demonstrated high accuracy, illustrating its capacity to adapt effectively to specialized domains using a moderately sized dataset. In contrast, GPT-4.0, through in-context learning and with a smaller dataset, achieved a significant R^2 value, proving its ability to efficiently extract and learn from limited information. These findings underscore the versatility of language models in extending their application beyond traditional linguistic tasks, offering valuable insights into their potential for advancing computational chemistry and facilitating interdisciplinary research between AI and chemical sciences.

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Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

DFT Study for the Reaction Pathway of Photocatalytic CO_2RR into Formic Acid using Ni-Perylene-Carbon Nitride Nanosheet (Ni-P-g-C_3N_4)

Mee Kyung Song, Young soo Kang*

Institute for Environmental and Climate Technology, Korea Institute of Energy Technology, Korea

Photocatalytic CO2 reduction reaction (CO2RR) into value-added oxygenated products is one of the most promising ways of solving climate warming change and energy crisis simultaneously. To get the oxygenated fuel products, it still remains great challenge in controlling both simultaneous sequential multi-electron/proton shuttling function through different transporting pathway, which determines the different intermediates and final products. To achieve this goal, we designed Ni-P-g-C3N4 catalyst for the highly selective production of formic acid (HCOOH) from photocatalytic CO2RR. As we know, CO2 to HCOOH is two electrons and two protons transferred process. To identify this selective reduction mechanism, we carried out DFT calculations using Dmol3. The CO2 adsorbed, intermediates and HCOOH adsorbed models have been constructed and we got the optimized structures and electronic properties. From the obtained free-energy profiles and free energy comparisons between reactant CO2 and key intermediates together with molecular orbitals, we can identify that the first proton was prone to be added firstly on the oxygen atom of CO2•- to form *COOH intermediate, rather than on the carbon atom of CO2•- to form H*COO intermediate. *Acknowledgement* The authors are grateful to the Leader Project at the Korea Institute of Energy Technology (KENTECH) funded by the Ministry of Science and ICT through the National Research Foundation of Korea (No. 2020R1A3B3079715), and the Korea Evaluation Institute of Industrial Technology (Alchemist Project 20018904, NTIS-141518011) through the Ministry of Trade, Industry and Energy, Korea. DFT calculation was supported by the National Supercomputing Center with supercomputing resources including technical support (KSC-2022-CRE-0286).

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Poster Presentation : **PHYS.P-90**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Kinetic and Thermodynamic Characterization of Antisense Oligonucleotide Binding to Target DNA

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A single nucleotide alteration within a gene, known as a single point mutation, is a major genetic variation, playing a crucial role in the emergence of various genetic disorders. Antisense oligonucleotides (ASOs) are short synthetic single-stranded oligonucleotides, which have been extensively utilized in gene therapy to regulate gene expression by targeting mRNA. Their target-specific binding characteristics of ASOs make them suitable for detecting single point mutations. However, current research lacks a comprehensive understanding of how ASOs interact with target DNA, particularly how these interactions vary with ASO lengths and temperatures. Our study aims to explore the optimal lengths of ASOs to enhance the discrimination of a single point mutation in target DNA. By positioning the mutation at the central region of ASO, we examined how ASO length affects the discrimination of the *KRAS* single-point mutation. Using single-molecule fluorescence resonance energy transfer, we investigated the real-time association and dissociation dynamics of ASOs for both the wild-type and mutant *KRAS* genes. Our findings revealed that both association and dissociation rates of ASOs were faster for mutant DNAs compared to wild-type DNA. Furthermore, the shorter ASOs exhibited enhanced binding and dissociation rates, with a maximum differentiation in binding affinities at a length of 9 nucleotides. Additionally, our temperature-dependent analysis uncovers the thermodynamic properties of ASO-gene interactions. This research identifies the optimal ASO length and temperature conditions for enhanced discrimination of single point mutations, contributing to refining genetic diagnostic and therapeutic methodologies based on ASOs.

Poster Presentation : **PHYS.P-91**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Deciphering the Molecular Mechanisms of Cas13a-RNA interactions: Binding, *Cis*-cleavage and *Trans*-cleavage

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Department of Chemistry, Chung-Ang University, Korea

The CRISPR system, known for its adaptive immunity in prokaryotes, has emerged as a powerful tool for gene editing due to its ability to precisely cleave DNA or RNA. CRISPR-Cas13a is one of the various CRISPR systems, and it specifically cleaves single-stranded RNA (ssRNA) as a complex with a guide RNA (gRNA). Despite the extensive exploration of Cas13a's potential in gene editing and diagnostic applications, the molecular mechanism underlying its RNA binding and cleavage processes remains elusive. In this study, we employed single-molecule Förster resonance energy transfer to investigate the real-time dynamics of RNA binding and cleavage by the Cas13a-gRNA complex. Our findings revealed a distinctive feature of Cas13a-gRNA, which could bind to its target RNA even without the presence of Mg^{2+} ions. However, this effective RNA binding does not lead to the anticipated cleavage of the target RNA, known as *cis*-cleavage. Interestingly, we observed a robust *trans*-cleavage activity, where Cas13a non-specifically cleaves nearby ssRNAs, in the absence of *cis*-cleavage. We further examined the effect of target RNA length on *trans*-cleavage activity, which revealed that longer target RNAs enhance the *trans*-cleavage rate, suggesting that the interaction of Cas13a with longer target RNAs might activate its *trans*-cleavage more effectively. In summary, our in-depth exploration of target RNA binding, *cis*-cleavage and *trans*-cleavage provides significant contributions to understanding the molecular mechanisms of Cas13a-RNA interactions.

Poster Presentation : **PHYS.P-92**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Theoretical study on the crucial role of metal coordination number in optimizing electrocatalyst activity of defective 2D Ru nanosheets.

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Low-dimensional metal nanostructures have attracted considerable research attention owing to their potential as catalysts and sensors. The universal importance of controlling the local structure was confirmed through a comparative study of Ru nanoparticles, which showed optimized hydrogen evolution reaction (HER) activity with an identical metal coordination number. In this study, we studied the dependence of Ru's HER activity on the surface coordination number based on density functional theory (DFT) calculation. According to the H adsorption energy with various coordination numbers, the Ru nanostructure with 2 defect sites near an active site shows the optimal HER activity. Based on the comparison of Volmer-Tafel energy diagram between a defected surface and a perfect surface, the defected surface has advantage with the stabilization of a dihydrogen Ru-(H2) intermediate that is a crucial intermediate for H-H bond formation. The density of states of Ru 4d states of perfect and defected surfaces shows that defected surfaces has an elevated d-band center that contributes to the thermodynamic preference of an associated dihydrogen intermediate to a dissociated dihydride intermediate. The coordination number defined by radial distribution function has a volcano relationship with H binding energy, which is a well-known HER descriptor, indicating the optimal number of defects can be suggested by theoretical calculations.

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Physical Chemistry
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Basis Set Extrapolation of HF/ROHF-DFT

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Modern computational chemistry uses a set of basis functions to represent wavefunctions and electron densities. By progressively increasing the size of the basis set and extrapolating the calculated physical properties, we can approach the complete basis set (CBS) limit, which represents the result when an infinitely large basis set is used. Using the CBS limit is both computationally efficient and accurate, as it allows us to extrapolate from smaller basis set results, minimizing computational cost while eliminating errors associated with finite basis sets. Meanwhile, electron densities derived by the Hartree-Fock (HF) method offer several advantages over self-consistent densities in DFT calculations. HF densities can be used in DFT calculations when self-consistent densities are physically inaccurate, a scheme known as HF-DFT. In this study, we show that HF-DFT is suitable for basis set extrapolation as it shows clear relationship between basis set size and energy. Furthermore, the CBS limit of HF-DFT shows a reduction in errors compared to unextrapolated results, suggesting a method for systematic improvement of HF-DFT. In spin-contaminated systems, however, HF-DFT fails to target the correct CBS limit because spin-contaminated densities do not represent the physically correct spin state. To ensure the elimination of spin contamination, we use densities derived by Restricted-Open Shell HF (ROHF), a variant of HF that correctly produces spin-squared values. Extrapolation of ROHF-DFT shows a clear correlation between basis set size and total energy. In particular, the CBS limit of ROHF-DFT significantly reduces the error compared to HF-DFT extrapolation results in spin-contaminated systems, validating the resolution of spin contamination problems.

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Poster Presentation : **PHYS.P-94**
Physical Chemistry
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Dynamical Simulation of Quantum Logic Gates based on Electronic Structure Calculations of Semiconductor Quantum Dots

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Gate-defined semiconductor quantum dots (QDs) form a useful platform for quantum computing due to their high controllability and fidelity in qubit operations. Computational studies on the electronic structure of the QDs may facilitate the discovery of new manipulation schemes for realizing efficient quantum logic gates. In this work, we have performed full configuration-interaction (FCI) calculations on coupled singlet-triplet (−) (S-T_-) qubits to study how the electronic energies and Hamiltonian parameters depend on the structure of the QD system. The QDs were modeled as truncated 2-dimensional harmonic potentials, and the electronic integrals were calculated by combining Fock-Darwin (F-D) states with the generating function method. The structure of the QD systems was tuned to exhibit tunnel couplings observed in the experiments. For both gallium (Ga) and silicon (Si) matrices, it was observed that the behavior of S-T_- qubits was not significantly affected by the size of the basis set, in terms of the avoided crossing, exchange couplings, and qubit energy gaps. In the future, we plan to use such computational capability to perform dynamical simulations of quantum logic gates employing S-T_- (singlet-triplet) qubits.

Poster Presentation : **PHYS.P-95**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Scaling Universality in Transport Distributions within Percolation Systems

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In our study, we focus on the electrical conductivity of percolating clusters in continuum and lattice spaces to identify the universality in transport distributions in percolation. We notice a consistent shift in the distribution shape of transport properties, transitioning from Gaussian to non-Gaussian near the percolation threshold, attributed to notable finite-size effects caused by the increasing correlation length of the percolating cluster. Specifically, at the percolation threshold, non-Gaussian transport distributions display universal finite-size scaling determined by a transport exponent. This finding suggests that the average and the distribution of transport properties adhere to the same universality class, governed by a common transport exponent. It offers insights into universal features in the distributions of various transport phenomena facilitated by percolating clusters, opening novel avenues for characterizing transport across a wide range of percolation-based systems.

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Physical Chemistry

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Characterizing Single Polymer Conformations from Coil to Globule Transitions

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Understanding the conformation of the smallest single polymer among various polymeric materials is essential for explaining properties in various systems. There are two scenarios for explaining this conformation behavior: (i) Effective two-body interactions, and (ii) Coil-to-globule transition. We carried out parallel tempering molecular dynamics simulations to observe characteristic temperatures, T_{cg}, for each scenario.First, the temperature decreases, conformation undergoes drastic change at the coil-to-globule transition. We numerically determine the $T_{cg,Rg}$ at which this transition takes place. Second, the heat capacity as a function of temperature forms a shoulder in the intermediate temperature region. We obtained second characteristic temperatures, $T_{cg,cv}$, using a hyperbola fit to these regions. We find that when N increases to infinitely, the two characteristic temperatures converge to the theta temperature, □ . Additionally, when N is a sufficiently large for a single polymer, we confirmed that both methods explain the conformational change of a single polymer well.

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Poster Presentation : **PHYS.P-97**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Utilization of reusable magnetic core-shell structured photocatalysts for the production of liquid fuels by CO2 reduction

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To reduce concentration of atmospheric CO_2, photocatalysts are utilized to convert CO_2 into useful chemicals. These catalysts are generally durable and reusable. But, to reuse them, an additional separation process such as centrifugation is required, leading to additional energy consumption. To remove this, fast and energy-efficient magnetic separation can be employed. rGO/NiO/CeO_2@SiO_2@Fe_3O_4 (RNCSF) composite were fabricated for a reusable and easily separable photocatalyst. Specifically, monodisperse Fe_3O_4 core microspheres were employed as templates for the deposition of additional layers. SiO_2 layer is coated onto the Fe_3O_4 core to prevent direct contact between magnetic core and the catalyst layer, using modified Stöber method. Subsequently, rGO/NiO/CeO_2 catalyst layer is deposited for effective CO_2 conversion. N-type CeO_2 catalysts are employed to activate the CO_2 to produce a liquid product. On the surface of CeO_2, CO_2 is adsorbed onto the oxygen vacancies created by solar light illumination. Following adsorption, activation of CO_2 takes place through the deformation of its linear structure, increasing the CO_2 reduction rate by lowering the activation energy. To suppress the charge recombination on CeO_2, p-type NiO was hybridized with CeO_2. Additionally, rGO was grafted onto NiO/CeO_2 heterostructure photocatalysts to facilitate a multi-electron transfer process. Above each catalyst were employed in CO_2 reduction experiments. The reduction products were quantified to assess CO_2 efficiency and selectivity.

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Physical Chemistry

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Structural Changes of Thioflavin T upon Intramolecular Charge Transfer Studied by Impulsive Stimulated Raman Spectroscopy

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Intramolecular charge transfer (ICT) has been of great interest in chemistry and related fields for many decades due to its potential applications, including molecular electronics, bio-imaging, etc. The structural changes of push-pull chromophores upon ICT have been widely investigated by numerous theoretical and experimental methods. Recently, we have shown the skeletal vibrational modes in the 1500-1650 cm^{-1} range, ν_{8a} and $\nu_{C=C}$, of the push-pull chromophores with π-conjugated backbones (stilbene, biphenyl, and styrylpyran) are sensitive to the structural changes of the backbones upon the ICT in the excited states. Femtosecond stimulated Raman spectroscopy (FSRS) with both high spectral ($^{-1}$) and temporal ($^{-1}$ range. Two kinetic components of ~370 fs and ~3.4 ps obtained from the population dynamics represent the structural changes of thioflavin T, where the vibrational modes at 211, 537, and 626 cm^{-1} showed the distinct kinetics from those at 473 and 508 cm^{-1}. The population dynamics and peak shifts in these vibrational modes are interpreted as structural changes, such as the bend of benzothiazole moiety and the twist of the dimethyl benzothiazole group with the theoretical calculations by TDDFT methods. The time-resolved vibrational probes of ISRS and FSRS may provide essential information toward understanding the chromophores' structural changes upon the ICT occurring in the ultrafast time scales.

Poster Presentation : **PHYS.P-99**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Lithiation of crystalline and amorphous silicon materials from molecular dynamics simulation with ReaxFF force fields

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With the rapid growth of the electric vehicle market, the demand for lithium batteries, the key energy storage device, is rapidly increasing. There are several issues that still need to be addressed, and increasing capacity is one of the most urgent among them. Silicon, which has a much higher capacity of 3700 mAh/g than graphite (375 mAh/g), is one of the most promising anode materials for next-generation secondary batteries. Silicon has a critical weakness compared to its high capacity: it undergoes significant expansion and contraction during charge/discharge cycles. This is a challenge that must be addressed to be adopted in practical batteries. In this study, we investigate the volumetric expansion of crystalline and amorphous silicon using molecular dynamics (MD) simulations. We performed molecular dynamics simulations of the reaction between silicon and lithium using the ReaxFF force fields. One of the main outcomes from simulation shows that crystalline silicon exhibits strong anisotropic expansion, while amorphous silicon undergoes nearly isotropic expansion.

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Physical Chemistry
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Excited-State Intramolecular Charge Transfer of Anthraquinones Confined in Reverse Micelles

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Investigation of excited-state intramolecular charge transfer (ICT) is crucial for its potential applications in solar energy conversion, photovoltaics, and fluorescence sensing, among others. The ICT dynamics of chromophores strongly depend on solvent properties, including polarity and viscosity, often accompanied by the structural changes of the electron donor or acceptor group. 1-Aminoanthraquinone (1AAQ) shows the ultrafast ICT in polar solvents with largely increased Stokes' shifts and decreased fluorescence quantum yields in steady-state absorption and emission measurements. Furthermore, the twist of the electron-donating amino group was suggested in femtosecond stimulated Raman measurements by the ultrafast dynamics (110 fs) in major vibration modes of 1AAQ, νC-N + δC-H (1200-1230 cm-1) and νC=O (1300-1330 cm-1). In this work, we present the ICT dynamics of anthraquinone derivatives, 1AAQ, 2-aminoanthraquinone (2AAQ), and 1-methylaminoanthraquinone (1MAAQ), confined in the core of the reverse micelles (RMs). The dependence of the ICT dynamics with structural changes of varying functional groups on several local properties (micropolarity and microviscosity) and electrostatic interactions with the surfactant head groups inside the RMs will be discussed based on the time-resolved absorption and emission measurements in ultrafast time scales.

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Physical Chemistry

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Diverse Quantum Interference Regime in Intramolecular Singlet Fission Chromophores with Thiophene-Based Linkers

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An array of thiophene-based π-conjugated linkers in covalently-linked pentacene dimers allows us to access diverse quantum interference (QI), modulating nonadiabatic coupling (NAC). Simulations show that structural isomerism in terms of S atom orientation can selectively alter NAC with marginal impacts on energies. Extended curly arrow rules reveal sensitive dependence of QI on SF linker topologies and connectivity, categorizing regimes of constructive, destructive, and previously unrealized in SF research, suppressed destructive QI (CQI, DQI, and SDQI, respectively). CQI of fused thiophenes with all trans S orientation becomes SDQI by insertion of at least one cis orientation, explaining 89 % NAC decrease. For the linkers belonging to SDQI regimes, NAC is highly sensitive to the number of mediating sulfur atoms. Changing the linking patterns modulates NAC up to 8-fold by changing operative QI. Our findings show that QI can rationalize and semi-quantitatively correlate to NAC between local exciton and multiexciton states.

Poster Presentation : **PHYS.P-102**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Simulation on Amorphous Solid State Electrolytes with Machine-Learning Potential

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All-solid-state battery (SSB) systems have gotten their attention for their safety and high energy density, and amorphous inorganic solid-state electrolyte (SSE) has emerged as one of the promising candidates due to its high ion conductivity and good chemical/electrochemical stability. Although the demand for predicting the properties of this type of material grows, traditional ab initio molecular dynamics (AIMD) simulation has its limitations on simulation size and time and this can affect the quality of prediction. Recently, Machine-Learning Potential (MLP) opened a new way of describing accurate interatomic interaction with less computational cost, thus expanding the boundary of scale limitations by training the model with the results of density functional theory (DFT). Among many types of MLPs, moment tensor potential (MTP) showed a remarkable result of accuracy with significantly less demand for dataset size and computational cost. In this study, we target to build an MLP model for lithium tetrachloroaluminate ($LiAlCl_4$) with high accuracy and low data cost, as well as the error benchmark acquired by comparing with a test case. With molecular dynamics (MD) simulation based on the trained MLP model, we compare density together with Li-ion diffusion coefficient at various temperatures and find the glass transition temperature ($T_g \approx$ 350K) of the material. By inspecting van Hove correlation function ($G_s(r, t)$), which shows the probability density of finding a particle in the vicinity of r at time t, we also discover the mechanism for Li-ion transportation mechanism below T_g , where Li-ion diffusing through the gaps between two tetrachloroaluminate ($AlCl^-$) tetrahedral structures.

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Poster Presentation : **PHYS.P-103**

Physical Chemistry

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Identification and Dynamics of Microsecond-Lived Charge-Carriers in Super-Stable $CsPbBr_3$ Perovskite Quantum Dots in SiO_x Matrix

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We present an analysis of the remarkable stability and photophysical dynamics of $CsPbBr_3$ perovskite quantum dots (PeQDs) embedded in an amorphous silica (SiO_x) matrix, highlighting their persistence in ambient conditions for over 300 days with minimal optical degradation. However, a notable compromise is observed in their photoluminescence efficiency. Time-resolved studies utilizing flash-photolysis time-resolved microwave conductivity (FP-TRMC) and time-resolved photoluminescence (TRPL) spectroscopy indicate that excitons within the $CsPbBr_3@SiO_x$ film exhibit a predominant decay time constant of 2.5 ns, whereas the average recombination lifetime of charge-carriers from FP-TRMC experiments is measured to be ~230 ns. This study further reveals the mechanism behind the long-lived charge-carriers, attributing to photoinduced electron transfer to the SiO_x matrix, leaving holes in $CsPbBr_3@SiO_x$, as evidenced by the usage of electron and hole scavengers. We also determined the hole mobility of 0.880 $cm^2\ V^{-1}\ s^{-1}$ of these nanoscale PeQDs, a crucial parameter for their application in optoelectronic devices. These results suggest that a SiO_x matrix successfully preserve PeQDs in humid environment over 300 days, while a moisture-resisting matrix can modulate the exciton dynamics and photoluminescence (PL) behaviors.

Poster Presentation : **PHYS.P-104**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Donnan equilibrium and electrostatic screening of confined electrolytes: A simulation study on the effects of their composition

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Recent surface force balance (SFB) experiments [1] have challenged our current understanding of the screening, such as the classical Debye-Hückel or mean-field theories: various concentrated electrolytes confined by mica surfaces show an unexpectedly long decay length of the force between surfaces (~ 10 nm), referred to as “underscreening.” Surprisingly, a universality was found in a cubic scaling relation of the decay length with ion size after proper normalization in both quantities with Debye screening length. However, the anomalous underscreening is still puzzling, as bulk theories with the primitive model of electrolytes [2] and all-atom simulations [3] have only found underestimated exponents (1-2) instead of the cubic scaling exponent. This poster presents our simulation results focusing on the confinement effect between two mica surfaces in SFB experiments. Electrolyte composition in the confined region could vary due to the Donnan equilibrium, depending on experimental conditions, such as the separation distance between two surfaces and bulk ion concentration. Our recent grand canonical simulation in the open environment [4] revealed that the Poisson-Boltzmann approach is still valid only with an additional parameter specifying the residual surface charge density after being screened by the surface-bound ions. In this work, we investigate the effect of electrolyte composition in the confined region on the electrostatic screening, exploring the possibility of the missing contribution to the cubic scaling relation found in the SFB experiments.References[1] A.M. Smith et al., JPCL 7, 2157-2163 (2016)[2] P. Cats et al., JCP 154, 124502 (2021)[3] S.W. Coles et al., JPCB 124, 1778-1786 (2020)[4] J. Kim et al., J. Phys. Chem. 159, 144802 (2023)

Poster Presentation : **PHYS.P-105**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Excited-state Proton Transfer of Green Fluorescent Protein Chromophores Investigated by Time-resolved Electronic and Vibrational Spectroscopy

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Excited state proton transfer (ESPT) is considered as one of the important photochemical processes due to various applications, including light-emitting materials, fluorescent probes, etc. Numerous experimental and theoretical investigations have focused on the details of ESPT dynamics to understand and manipulate important photochemical processes. Green fluorescent protein (GFP) from the jellyfish Aequorea victoria is one example, as it has been extensively investigated as a prominent fluorophore due to its high fluorescence quantum yield and non-toxicity in vivo. Intermolecular proton transfers between the GFP chromophore and water molecules in the excited state are considered crucial in the strong fluorescence of GFP. However, the details of the ESPT in the GFP chromophore and its analogues and the relationship between the ESPT dynamics and chromophores' structural changes are not yet clear. In this work, we report the ESPT of a GFP chromophore, 4-(4-hydroxybenzylidene)-1,2-dimethyl-1H-imidazol-5(4H)-one (p-HBDI) and an analog, 4-(2-hydroxybenzylidene)-1,2-dimethyl-1H-imidazol-5(4H)-one (o-HBDI) by femtosecond transient absorption and stimulated Raman spectroscopy. The ESPT dynamics of the GFP chromophores will be reviewed in terms of the excited electronic transitions and corresponding structural changes of the chromophores.

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Poster Presentation : **PHYS.P-106**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Density and Dispersion Corrected Density Functional Theory

<u>Minhyeok Lee</u>, Byeongjae Kim[1], Youngsam Kim[1], Eunji Sim[1,*]

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Density functional theory (DFT) is a cornerstone of computational chemistry, offering a balance between accuracy and computational efficiency. Despite its widespread use, improving DFT functionals systematically remains a challenge. Our research introduces density and dispersion corrected density functional theory (DC^2-DFT), an dual-calibration approach designed to address both functional inaccuracies and density-driven errors in DFT calculations. Applying DC^2-DFT across 14 different functionals, including GGA, mGGA, and hybrids, we demonstrate its effectiveness and versatility across diverse chemical systems, such as GMTKN55, WATER27, Bauza, and the large molecular datasets L7 and S6L. DC^2-DFT hinges on resolving two major obstacles in DFT: correcting density-driven delocalization errors and mitigating dispersion errors through strategic training set selection for parameterization. This methodology is grounded in the principles of density-corrected DFT, underscoring the importance of dual-calibration in guiding DFT development towards more accurate and reliable predictions.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **PHYS.P-107**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancing Molecular Design Through Explainable Deep Learning Models

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

Innovative materials design requires accurate prediction of molecular properties based on an understanding of molecular structure-property relationships. Many conventional methods offer limited insights into prediction of molecular properties. For example, the Woodward-Fieser rules are used to predict only absorption and emission wavelengths of conjugated molecules. In this work, we introduced an advanced approach leveraging explainable deep learning optical spectroscopy (DLOS) to overcome such limitations. By employing the integrated gradients method within a DLOS framework, we quantitatively analyzed the contribution of functional groups and solvents to seven optical properties, including absorption peak position and bandwidth, extinction coefficient, emission peak position and bandwidth, photoluminescence quantum yield, and emission lifetime. The attributions of 54 functional groups and 9 solvent molecules to seven optical properties were properly quantified and were shown to be used to estimate seven optical properties of organic molecules as in the Woodward–Fieser rule. This methodological advancement could not only broaden the scope of the Woodward−Fieser rules but also facilitate a more nuanced manipulation of molecular structures for optimal optical properties. The details and performance of explainable DLOS will be presented.

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Poster Presentation : **PHYS.P-108**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Comparison of The Performance of HF-DFT with vdW-functionals in Condensed Phase Calculations

<u>Youngsam Kim</u>, Eunji Sim*

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Density functional theory (DFT) has been a commonly used method for solving electronic structure problems due to its high precision and cost-effectiveness. Unfortunately, the limited understanding of the exact exchange-correlation potential as a function of density makes it difficult to find a universal solution with the limitation that the accuracy depends on the approximation. A major shortcoming of DFT calculations in the condensed phase is that long-range interactions are not accurately predicted. To address this, approximations such as opt-vdW and vdW-DF, which explicitly account for the dispersion interaction, are generally used. However, this work shows that these approximations are system-dependent and tend to overestimate the adsorption energy in surface interaction and cohesive energies in molecular crystals. We then demonstrate that this can be overcome by using Hartree-Fock DFT (HF-DFT) with a sophisticated dispersion correction. By comparing the performance of HF-DFT with that of vdW-functionals and the general approximations in condensed phase calculations, we demonstrate the transferability of HF-DFT and suggest its potential as a generally applicable tool for such calculations.

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Poster Presentation : **PHYS.P-109**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Optical activity detection via repetition rate multiplication of an optical frequency comb

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Optical frequency comb is a high precision spectroscopic technique based on the atomic clock that has brought revolutionary insights to various fields of physical chemistry. Here, we demonstrate doubling of the repetition rate of Ti:Sapphire optical frequency comb, that originally operates at 80 MHz, by adopting an additional optical path length which results in a quasi-160 MHz system. This scheme allows for separate modulation of each optical path before combining them. In our case, polarization optics are adjusted on each path so that an alternating pulse sequence of right- and left-handed circular polarization light is generated. Using synchronized detection referenced by the atomic clock, the split pulses can be registered with a single channel detector and comparatively analyzed by separating even and odd datasets. This method can be regarded as a divergent type of self-referenced detection that is distinguished temporally, i.e. one pulse serves as a reference to the one directly following it. The configuration can be applied and utilized in cases where the relative intensity between pulses with different handedness varies with time, such as the measurement of time-resolved optical activity.

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Poster Presentation : **PHYS.P-110**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Hartree-Fock DFT for Dipole Moments

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The dipole moments of molecules are crucial for understanding and predicting the physical, chemical, and biological behavior of substances. Dipole moments are also used to describe long-range electrostatics in molecular dynamic simulations. Since the dipole moments can be obtained theoretically through numerical derivatives of energy to the electric field, the accuracy of the electronic structure calculations is important. Density Functional Theory (DFT) has significantly advanced the field of quantum chemistry by enabling scientists to analyze molecular systems and predict their properties with computational efficiency and accuracy. However, previous studies have demonstrated that DFT can be affected by density-driven errors, and in this case, DFT with Hartree-Fock density (HF-DFT) can be a practical solution to get improved results in energies and energy differences of various chemical reactions. Not only in terms of the energy but also in terms of the dipole moment, the HF density exhibits significantly different behavior from the self-consistent density of systems where the DFT has large errors. We examine the error of HF-DFT with each lung of the Jacobs ladder. A standard procedure has been developed to evaluate dipole moment sensitivity when using HF density instead of self-consistent density. The question of why HF-DFT is physically more valid with dipole moment curves corresponding to non-equilibrium states is also discussed.

Poster Presentation : **PHYS.P-111**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Intramolecular Charge Transfer of Stilbazolium Derivatives Studied by Time-resolved Vibrational Spectroscopy

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Intramolecular charge transfer (ICT) in the exited state occurs between the electron donor and acceptor groups connected by the pi bridges, and chromophores’ structural changes, such as the twist of the donor or acceptor group, are often observed in the ultrafast time scales. Many researchers have recently investigated the ICT dynamics of numerous chromophores with varying electron donor/acceptor groups and π-bridges by time-resolved electronic spectroscopy and theoretical calculations based on time-dependent density function theory (TDDFT) methods. Time-resolved electronic probes are inherently insensitive to the chromophores’ structural changes. Thus, time-resolved vibrational probes, such as time-resolved Raman or infrared spectroscopy would be essential in the exploration of the structural modifications in the excited states. In this work, we compare the ICT dynamics of stilbazolium derivatives with varying steric hindrance for the internal rotation of electron donor or acceptor group by femtosecond stimulated Raman spectroscopy (FSRS). The structural changes of 4-N,N-diethylamino-4'-N'-methylstilbazolium tosylate (p-DEST) with the twist of diethylaminophenyl group are represented by the skeletal vibrational modes, v(8a) and v(C=C) in the 1500-1650 cm-1 range. On the other hand, a stilbazolium derivative with the steric hindrance for electron donor’s twist, of 4-N,N-diethylamino-2'-N'-methylstilbazolium tosylate (o-DEST) shows no such changes in the skeletal vibrational modes of styrylpyridinium backbone. The structural changes of stilbazolium derivatives with the ultrafast ICT in the excited state are supported by the TDDFT simulation results.

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Physical Chemistry
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Synthesis and Photophysical Studies on Organic D-A Charge-Transfer Complex with SWIR Emitting Bandgap by Adjusting the Rotation Angle of D-A Configuration

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

Organic donor-acceptor (D-A) charge transfer complexes (CTCs) are representative organic semiconductors, due to their solution processability and economic advantages. Their bandgap tuning is achieved by simply controlling the energy levels of each component (D and A) and their D-A packing structures. Especially, due to their low absorption and emission efficiency, there is a need to investigate NIR CTCs using a simplified model system.In this study, we fabricated NIR CTCs composed of TCNQ as an acceptor, along with carbazole (Cz) derivatives as donors, having comparable HOMO levels but different orientations of Cz units. All CTCs showed CT absorption and emission up to SWIR range, with different bandgaps according to their Cz-TCNQ configurations. Computational analysis showed as the rotation angle between Cz and TCNQ increases, the forbidden lowest transition becomes allowed, therby resulting in lowered optical bandgap.

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Poster Presentation : **PHYS.P-113**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Rebound kinetics of carbon monoxide with heme proteins using time-resolved infrared spectroscopy

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Department of Chemistry, Pusan National University, Korea

Time-resolved vibrational spectroscopy was used to study the rebinding dynamics of CO to cytoglobin (Cgb) and myoglobin (Mb) after photodeligation of the corresponding CO-bound protein in aqueous solution at 273 K. When excited with a 532-nm photon, carbon monoxide dissociates from heme proteins immediately (< 0.2 ps), and the ground-state bleaching of heme protein-bound CO has three conformations (A0, A1, and A3). This ground-state bleaching of heme protein-bound CO is related to distal histidine. Histidine, along with other amino acid residues, contributes to the overall structure and stability of the heme pocket. The arrangement of these residues influences the binding and release of ligands, such as oxygen, carbon monoxide, and nitric oxide. We have studied the dynamics depending on these different conformations of distal histidine.

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Poster Presentation : **PHYS.P-114**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Novel Subgroup-wise Attention Network for Interpretability

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

With the advancement of deep learning (DL) methods, there has been a growing interest in utilizing DL models for the development of new materials. However, despite the remarkable performance of DL models, their interpretability remains a significant concern, particularly in materials science where predicting molecular properties based on the molecular structure-property relationships is crucial. Although attention mechanisms have been employed to explain the areas of focus within the DL models, their interpretability is still limited. In this study, we addressed this limitation by proposing a novel approach termed interpretable subgroup-wise attention network (ISA-Net), which incorporates subgroup-wise attention with advanced techniques to elucidate the molecular structure-property relationships. Specifically, we introduced a novel fragmentation algorithm and the PN method to facilitate the implementation of the ISA-Net. Unlike traditional attention methods, which primarily indicate the areas of focus without elucidating the contributions of individual moieties, the ISA-Net allows us for the quantification of the contributions of moieties. Using a comparative analysis with traditional attention methods and group contribution methods, we demonstrate that the ISA-Net significantly enhances interpretability while maintaining comparable accuracy levels. Our findings underscore the efficacy of the ISA-Net in providing meaningful insights into the molecular structure-property relationships, thereby advancing the interpretability of the DL models in materials science.

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Poster Presentation : **PHYS.P-115**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Formation of Alkali-Halide Cluster Ions with Aza-Crown Ethers

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Ionic clusters, formed through covalent and non-covalent interactions, play crucial roles in electrolyte systems within diverse electrochemical devices. Gas-phase mass spectrometry (MS) and ion mobility spectrometry-mass spectrometry (IMS-MS) have emerged as indispensable tools for exploring the intrinsic properties of these clusters in solvent-free environments. By combining collision cross-section (CCS) values from IMS-MS with Density Functional Theory (DFT) calculations, structural predictions are facilitated. Additionally, Collision Induced Dissociation (CID) provides insights into comparative ionic bond strengths within clusters.This study focuses on investigating the behavior of ionic clusters formed by alkali metal ions confined by aza-crown ethers as binders. Through IMS-MS and theoretical calculations, we confirmed the presence of monomer clusters (aza-crown ether + M^+) and dimer clusters effectively entrapping various anions. Our findings reveal size-dependent interactions between alkali metal ions and aza-crown ethers, elucidating the ability to control binding strength between ions. Low-energy CID further substantiates the divergence in cationic characteristics depending on the binder, highlighting the utility of our approach in understanding and manipulating ion-binding interactions.

Poster Presentation : **PHYS.P-116**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Structures of $(Li^+I^-)_nLi^+$ Cluster Ions Solvated by Ethylenediamine

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Lithium has widespread applications in daily life, particularly in lithium-ion batteries. Therefore, understanding the formation and solvation properties of ionic clusters containing lithium ions is crucial for influencing ion transport behaviors. In this research, we examined $(Li^+I^-)_nLi^+$ cluster ions in solvation with ethylenediamine using electrospray ionization–ion mobility spectrometry–mass spectrometry (ESI–IMS–MS). Solvation complexes were generated through two methods: one involved ESI of a solution comprising LiI and ethylenediamine, and the other employed ESI of a LiI solution with ethylenediamine vapor produced by N_2 bubbling. IMS–MS enabled the characterization of the components and structures of solvation complexes formed by each method. While complexes of smaller size $(n^+I^-)_nLi^+$ ionic clusters with organic molecules such as ethylenediamine. Furthermore, this research identified the mechanisms for the formation of solvation complexes in different methods, providing insights into solvation studies conducted in both solution and gas phases.

Poster Presentation : **PHYS.P-117**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Rotational Isomerization of $CF_3CF_2CF_2$ Radical in solution

Seongchul Park, Juhyang Shin, Manho Lim[*]

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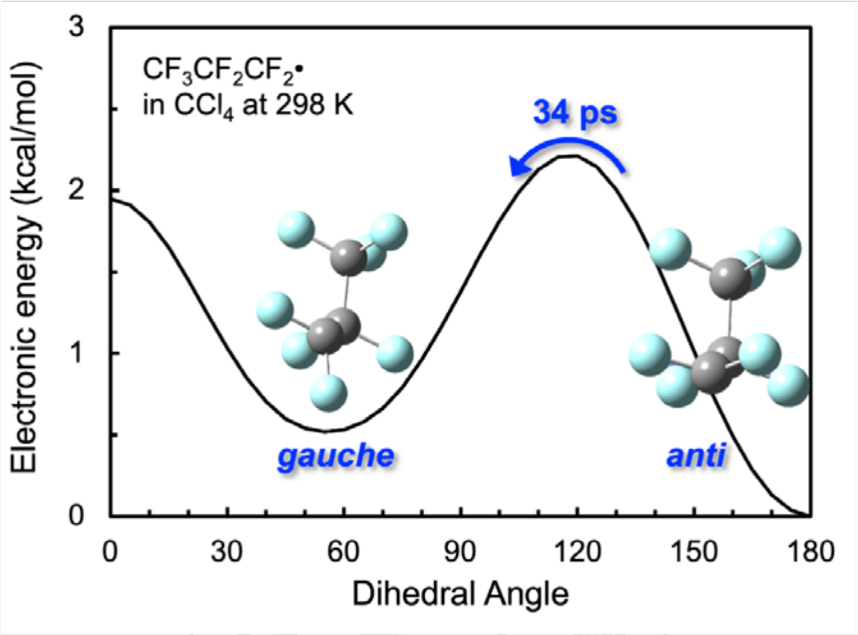
The photodissociation dynamics of CF3CF2CF2I dissolved in CCl4 solvent at 293 K were studied using time-resolved infrared spectroscopy after excitation by 267 nm photons. Infrared spectral analysis shows that CF3CF2CF2I has two stereoisomers at room temperature: anti-CF3CF2CF2I (84%) and gauche-CF3CF2CF2I (16%). However, when the I atom is dissociated from the parent, the difference in free energy between the anti-CF3CF2CF2 and gauche-CF3CF2CF2 radicals narrows to only ~0.4 kcal/mol, giving 46% and 54%, respectively. This indicates that the excess of anti-CF3CF2CF2 formed by the dissociation of the I atom relaxes to a level of 46%, which is the equilibrium level. We observed the kinetics of anti-CF3CF2CF2 and gauche-CF3CF2CF2 radicals by observing the C-F stretching mode of the radical, and the rotational isomerization time of the radical was measured to be 34 ps. This is consistent with the expected result of 32 ps from Kramer theory based on DFT calculations. The rotational isomerization time of carbon-carbon single bonds is rarely reported, but they are crucial in determining the stereochemistry of products in chemical reactions. Based on our measurements, we expect to establish a method for predicting the time of rotational isomerization of other similar molecules.


3
2
1
0
Electronic energy (kcal/mol)
0
30
60
90
120
150
180
Dihedral Angle
$CF_3CF_2CF_2\bullet$
in CCl_4 at 298 K
34 ps
gauche
anti

Poster Presentation : **PHYS.P-118**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

New methodological Fischer-Tropsch chemistry

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Fischer-Tropsch (F-T) chemistry is a crucial reaction for transforming syngas into hydrocarbon products. However, it requires significant energy input due to the high pressure and temperature conditions. In recent research, an alternative approach has been explored, utilizing electrochemistry with electrochemical catalysts under ambient conditions. In this study, we present the results of F-T chemistry conducted at ambient temperature and pressure.

Poster Presentation : **PHYS.P-119**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Isomerism Introduced by Altering Connectivity between Anthracene Chromophores

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9,9-bianthracene (BA) is a prototype material for studying symmetry-breaking charge transfer (SBCT) due to its structural simplicity and its torsion-driven mechansims in the reaction. Its orthogonal structure typically results in a mono-exponential decay due to the torsional rigidity induced by steric hindrance of adjacent hydrogen atoms, suggesting the uniformity of its conformers. Recently, the studies of bianthracene derivatives like 2,9’-bianthracene and 1,9’-bianthracene yielded similarities to BA's SBCT character, primarily because of their similar orthogonal structures. Here, this study introduces 9,9’,10,10’-Tetraphenyl-2,2’-bianthracene (TPBA), exhibiting a markedly different geometry and excited-state dynamics compared to BA. The reduced steric hindrance in TPBA facilitates a tendency towards planarity, enhancing short-range exciton coupling. Quantum mechanical calculations have revealed two distinct local energy minima in TPBA, demonstrating dihedral angles of 35° and 141°, corresponding to trans and cis conformers. Utilizing time-resolved fluorescence spectroscopy, we identified distinct emissive spectra and fluorescence lifetime for these conformers, specifically 5 ns for trans and 30 ns for cis. Further analysis showed that the trans conformer exhibits a higher radiative and non-radiative rate compared to the cis conformer. These differences are supported by TD-DFT calculations, highlighting a fourfold greater oscillator strength for the (0,0) transition in the trans conformer. Additionally, potential energy surface scans based on DFT/TD-DFT revealed a higher torsional barrier in the S1 state of the cis conformer, limiting its torsional degree of freedom and resulting in a decreased non-radiative decay rate.

Poster Presentation : **PHYS.P-120**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

The Impact of Oligothiophene Linkers in Heterogeneous Triplet Formation Pathways of 6,6’-Linked Pentacene Dimers

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Singlet Fission (SF), a phenomenon where one singlet exciton generates two triplet excitons, is exclusive to organic semiconducting materials[1]. This phenomenon has been attracting considerable attention due to its potential to exceed the Shockley-Queisser limit through carrier multiplication in photovoltaics[2,3]. A molecular dimer covalently bonded serves as the basic model for understanding SF mechanisms because it consists of two closely interacting chromophores, thus capable of yielding two excitons[4]. In this research, we explored the intramolecular SF dynamics of pentacene dimers linked by 6,6'-connections with various oligothiophene linkers to elucidate the role of linkers in controlling SF pathways. Through femtosecond transient absorption (TA) measurements, we found that SF behaviors are heavily influenced by the number of oligothiophenes in the linker and the presence of ring fusion. Furthermore, we selectively excited specific conformers by targeting the red-edge of the absorption band to uncover the effects of conformational heterogeneity on SF efficiency. Finally, we differentiated between two types of triplets generated through distinct pathways by analyzing TA kinetics across femtosecond to microsecond time scales. Overall, we anticipate that our investigation can offer molecular design principles for enhancing intramolecular singlet fission efficiency.References[1] M. B. Smith, J. Michl, Chem. Rev, 2010, 110, 6891.[2] W. Shockley, H. J. Queisser, J. Appl. Phys, 1961, 32, 510.[3] M. C. Hanna, A. J. Nozik, J. Appl. Phys, 2006, 100, 074510.[4] N. V. Korovina, N. F. Pompetti, J. C. Johnson, J. Chem. Phys. 2020, 152, 040904.

Poster Presentation : **PHYS.P-121**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhanced Chemical Stability of Radical Cations in Carbazole-based Diketopyrrolopyrrole Derivatives

Jungjin Park, **Sanchari Debnath**[1], **Vithobha Hugar**[1], **Ram Kumar Canjeevaram Balasubramanyam**[1], **Woojae Kim**[*], **Satish Patil**[1,*]

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[1]*Solid State and Structural Chemistry Unit, Indian Institute of Science, India*

Synthesis and stabilization of organic radical ions continue to attract immense interest due to their intriguing optical, electronic, and magnetic properties. However, stable radical cation generation under ambient conditions provides significant challenges due to their high reactivity. One of the notable strategies to mitigate these challenges is the construction of D-π-A conjugated systems, where incorporating a suitable donor helps stabilize the radical cation. Herein, we report unprecedented stable radical cation formation in diketopyrrolopyrrole (DPP) derivatives with 2- and 3-substituted carbazoles (2CzDPP and 3CzDPP) in the presence of external chemical stimuli. Further, the radical cation of 3CzDPP shows enhanced stability than 2CzDPP owing to the exceptional donating ability of 3-substituted carbazole, decisively established using spectroscopic and electrochemical characterizations. Notably, our work presents an elegant demonstration of donor-substituted DPP core as a new class of derivatives for stable radical cation generation, thereby providing a strategy for systematically controlling radical species.

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Poster Presentation : **PHYS.P-122**
Physical Chemistry
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Unraveling the chirality transfer from chiral molecules to plasmonic nanoparticles.

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Plasmonic chiral nanomaterials have emerged significant attention as promising materials for various optical technologies, including catalysts, chiral sensing, and medical imaging. Here we employed chiral molecules as chiral sources to effect chirality transfer from achiral to chiral states. Furthermore, we observed that as chiral molecules aged, they formed disulfide bonds, which negatively affected the transmission of chirality. Characterization techniques such as Circular Dichroism (CD) and Scanning Electron Microscopy (SEM) were utilized to confirm the property of chiral transfer. In this study, we systematically investigate the mechanism of chirality transfer and synthesize chiral nanoparticles through diverse approaches employing chiral sources. This comprehensive study contributes to the understanding of the synthesis mechanisms of chiral nanoparticles and offers interesting prospects for the advancement of chiral nanoparticle synthesis.

Poster Presentation : **PHYS.P-123**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Solvent and Fluence-Dependent Exciton Dynamics in One-Dimensional Perylene Bisimide H-Aggregates

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Supramolecular dye assemblies, particularly those formed by perylene bisimide dyes, hold tremendous potential for applications in optoelectronics. Thus, understanding the complex exciton dynamics within these assemblies, especially in H-type aggregates which can be a good candidate for light-harvesting application due to the generation of long-lived excitons, considered critical in photochemistry. In this study, we investigate the comprehensive dynamics of delocalized Frenkel exciton, localized excimer and charge separation of π-π stacked perylene bisimide aggregates. Through analysis of femtosecond and nanosecond transient absorption spectra, we demonstrate that in helical π-stacked aggregates, the initial delocalized Frenkel exciton go through charge separation process within few picoseconds and undergoes relaxation pathways, such as charge recombination process within tens of picoseconds. Also, we revealed the existence of exciton-exciton annihilation (EEA) channel in long axis of helical aggregates through pump fluence dependence transient absorption experiments. We figured out EEA process take place within hundreds of femtoseconds before the charge separation process occurs, so the EEA process can affect the processes that follow. Our experimental findings reveal novel insights into the delocalized Frenkel exciton dynamics and exciton annihilation channel in helical π–π stacks of perylene bisimide dyes. This study contributes to the ultrafast exciton dynamics of molecular H-aggregates, crucial for advancing material performance in various applications, and underscores the importance of understanding exciton behavior in dye self-assemblies.

Poster Presentation : **PHYS.P-124**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Bioinformatic Analysis of Protein Structures Using Contact Map Formalism

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Structural information of a protein is the key to understanding its function. Various experimental approaches have been developed to determine protein structures, leading to the construction of a database that contains hundreds of thousands of protein structures. The extensive database can be used to uncover the principles governing protein folding and design. Previous studies indicate that the topological information of protein structures is often sufficient to extract these fundamental principles. One representation of protein topology is a contact map (CM), which is a 2-dimensional matrix that contains information about the non-covalent contacts between residues in a protein. In this study, we tested several quantities (such as trace and element sum) derived from a CM to characterize a protein structure, and found that CMs and their derived quantities can reveal the structural and evolutionary diversity of proteins. We anticipate that these measures, based on CM, have the potential to serve as a straightforward and effective proxy for evaluating the evolvability of proteins. Furthermore, they can play a crucial role in facilitating the de novo design and engineering of biomolecules.

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Poster Presentation : **PHYS.P-125**
Physical Chemistry
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Towards Accurate Determination of Binding Free Energy Using Molecular Dynamics Simulations

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The binding affinity between a protein and its ligand partner is crucial for predicting medicinal effects in pharmacology. To computationally obtain binding affinity, several MD-based methods have been developed, and umbrella sampling (US) is one among them. In a typical US approach, the conformations along the reaction coordinate are selected at regular intervals. An external potential is then applied to each conformation to constrain the system around the target conformation, followed by MD simulations for extensive sampling. The contribution of this external potential to the population is later subtracted, resulting in the free energy profile along the reaction coordinate. By comparing the free energies of the bound and unbound conformations, one can derive the binding free energy, thereby yielding the binding affinity. However, it has been reported that the binding affinity largely depends on the path of dissociation and can also be influenced by other factors, such as the initial structure, the number of samples, and the sampling method. This makes it challenging to use the US for accurate determination of binding affinity.In this work, we improved the conventional US pipeline to obtain a more accurate and reproducible binding affinity for a protein-ligand complex. We tested several dissociation paths and devised an unambiguous dissociation path. The free energy derived from this pathway by the US was further supplemented by additional free energy terms, accounting for the thermodynamics of initial and final structures, resulting in corrected free energy. We believe that our work will pave the way to de novo drug design, which requires the accurate binding affinity of a protein-ligand system.

Poster Presentation : **PHYS.P-126**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Investigating Solvation Structures in Lithium-Ion Batteries: A Spectroelectrochemical Approach

Jungmin Park, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

Lithium-ion batteries (LIBs) have become indispensable in our modern society, powering everything from portable devices to electric vehicles. Despite extensive research focused on improving battery materials to enhance battery life, safety, cost, and charging efficiency, the intricate molecular mechanisms within these batteries, particularly those related to solvent interactions, remain largely unexplored. Solvents play a crucial role in lithium-ion transport, desolvation, intercalation processes, and the formation of the solid electrolyte interphase (SEI) on the electrode surface. While solvation structures of bulk electrolytes have been examined in our laboratory, observations at the diffusion layer and electrode surface—areas critical in actual battery environments—have not been conducted. To bridge this gap, we have developed a hole-processed spectroelectrochemical cell designed to mimic real battery conditions. This setup has allowed us to observe the carbonate solvent's free and bound peaks, both in the bulk solution and near the electrode, enabling us to determine the coordination number and, consequently, compare the solvation structures at these two locations. Our findings provide valuable insights into the solvation dynamics within LIBs, offering potential pathways for optimizing battery performance and longevity by tailoring electrolyte and electrode interfaces for enhanced ion transport and stability.

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Poster Presentation : **PHYS.P-127**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Molecular Dynamics Study on the Mechanical Deformation of Ionic Liquid Treated PEDOT:PSS Film

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Poly(3,4-ethylenedioxythiophene):poly(stryrenesulfonate) (PEDOT:PSS) is the most promising material for stretchable electronic components because it is stable, transparent and solution processable. However, the pristine PEDOT:PSS thin film has limited electrical conductivity (

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Poster Presentation : **PHYS.P-128**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Molecular Dynamics Simulations of DNA Rotaxanes

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DNA rotaxanes, mechanically interlocked with circular and linear axle double-stranded (ds) DNA, are widely used in molecular walkers, biosensors, etc. Here, we studied the structure and dynamics properties of rotaxanes composed of dsDNA using atomistic molecular dynamics simulation. We used 70-90 base pair (bp) AT/AT sequences because of shape distortion induced by torsional stress to determine the extent to which the structural and dynamics properties depend on the shape of circular dsDNA. We calculate the shape of circular dsDNA, intermolecular distances, and tilt angles for structural properties. Also, we show the translation and rotational mean square displacement of circular dsDNA for dynamic properties. Our investigation is the shape distortion of circular dsDNA causes the distance between minicircle and axle closer and brings an increase in translation with decrease in toroidal rotation.

[1] Y. Song, J. S. Kim, Structure and dynamics of double-stranded DNA rotaxanes, *Nanoscale*, Accepted, DOI: 10.1039/D3NR05846H

Poster Presentation : **PHYS.P-129**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Phase Separation of Amino Acid Derivatives and Water: Molecular Dynamics Study

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Biological systems utilize the phase separation of biomolecules in cells. This mechanism plays a crucial role in regulating biological reactions and facilitating the spatiotemporal separation of biomolecules in vivo. Phase separation can induce the local accumulation of particular molecules, hence acting as a catalyst for biological reactions. Also, phase separation often occurs as an intermediate step in the process of liquid fibrillization. Thus, it is important to understand the molecular principles of biomolecular phase separation.To obtain insight into biomolecular phase separation, we employ a simple model system that can undergo phase separation and simulate its phase behavior using molecular dynamics (MD) simulations. The key player in our model system is an amino acid protected by the Fmoc group. The Fmoc-protected amino acid contains both hydrophobic (Fmoc) and hydrophilic (amino acid) groups, and the balance between them can be easily controlled by using different side chains. When mixed with water, the Fmoc-protected amino acid exhibits rich phase behaviors, depending on its side chain. In this work, we focus on two systems, Fmoc-isoleucine and Fmoc-leucine, whose chemical structures and properties are quite similar, yet their collective behaviors show drastic differences experimentally. By using replica-exchange MD (REMD) combined with the slab method, we could successfully reproduce the experimental results and explain their molecular details.Through this research, we have discovered that subtle structural differences can result in entirely distinct collective behaviors. We anticipate that this work will pave the way for a more comprehensive understanding of molecular behaviors in both simple molecules and biomolecules.

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Poster Presentation : **PHYS.P-130**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Characterization of Nanoscale Spatial Heterogeneity in Inter- and Intra-Chain Entangled Polymer Networks Using the Random Barrier Model

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Single-molecule tracking (SMT) is a powerful method for characterizing diffusion behavior of probe molecules in a complex media. In our previous report, we evaluated the dependence of affinity with solvent on chain conformation and structural heterogeneity in highly crowded PMMA solution using SMT. We discovered abnormal long-range hopping of N,N'-dipentyl-3,4,9,10-perylenedicarboximide (pPDI) fluorescent probes in van Hove distributions, as well as the existence of mesoscopic region according to Gaussian and exponential crossover point displacement (Δxc). In this poster, we characterize the structural heterogeneity and the average size of mesoscopic region in the inter- and intra-chain entangled polymer network as motivated by random barrier model. By adjusting the jump threshold randomly, the distribution of waiting time the pPDI spends in one region before hopping to another is obtained. When the average activation energy (Ec) required to cross the random barrier is maximum, the jump threshold is equivalent to the previously determined Δxc, indicating another indicator that can be used to calculate the average size of the mesoscopic region where the diffusion behavior of pPDIs shows Brownian. Furthermore, for the same swelling ratio, the region size inside the intra-chain entangled network is less than that within the inter-chain entangled network, validating the stronger spatial heterogeneity according to the self-entangled chain conformation. This study indicates that the structural characteristics of polymer networks have a significant impact on mass transfer in soft matter systems.

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Poster Presentation : **PHYS.P-131**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Production of Single-Phase High-Entropy Alloys (Au, Ru, Ir, Pt and Pd) via CO_2 Laser for Hydrogen Production Through Seawater Electrolysis

Chae Eun Park, Dong Hyeon Lee, Theerthagiri Jayaraman, Myong Yong Choi*

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In this study, we synthesized a low Pt-based high entropy alloy (HEA) that formed shapes, both non-flowered and flowered, with sizes of 250 nm or more by irradiating a continuous wave (CW) CO_2 laser. The synthesized HEA demonstrates outstanding hydrogen production performance despite its out-of-size materials, showcasing high electrocatalytic activity. The electrochemical results revealed that HEA-60 exhibits remarkable electrocatalytic performance for the hydrogen evolution reaction (HER) with a low overpotential of 37, 34, and 45 mV at 10 mA cm^{-2} in 1.0 M KOH, 1.0 M KOH + 0.5 M NaCl, and 1.0 M KOH + real seawater electrolyte, respectively. Moreover, the overall seawater splitting process requires a low cell voltage of 0.24 V to achieve a stable current density of 10 mA cm^{-2} with excellent stability. Although HEA is composed only of noble metals, its size is on the μm scale to provide general catalytic activity. Despite containing a relatively small amount of Pt compared to other metals, it exhibits excellent activity. This study presents a simple and effective approach to synthesizing HEAs through entropy alloy engineering that could be utilized in energy and electrocatalytic applications.

Poster Presentation : **PHYS.P-132**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Triphenylphosphonium-Functionalized Dimeric BODIPY-Based Nanoparticles for Mitochondria-Targeting Photodynamic Therapy

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The dimerization of boron dipyrromethene (BODIPY) moieties is an appealing molecular design approach for developing heavy-atom-free triplet photosensitizers (PSs). However, BODIPY dimer-based PSs generally lack target specificity, which limits their clinical use for photodynamic therapy. This study reports the synthesis of two mitochondria-targeting triphenylphosphonium (TPP)-functionalized meso-β directly linked BODIPY dimers (BTPP and BeTPP). Both BODIPY dimers exhibited solvent-polarity-dependent singlet oxygen (1O2) quantum yields, with maximum values of 0.84 and 0.55 for BTPP and BeTPP, respectively, in tetrahydrofuran. The compact orthogonal geometry of the BODIPY dimers facilitated the generation of triplet excited states via photoinduced charge separation (CS) and subsequent spin–orbit charge-transfer intersystem crossing (SOCT–ISC) processes and their rates were dependent on the energetic configuration between the frontier molecular orbitals of the two BODIPY subunits. The as-synthesized compounds were amphiphilic and hence formed stable nanoparticles (~36 nm in diameter) in aqueous solutions, with a zeta potential of ~33 mV beneficial for mitochondrial targeting. In vitro experiments with MCF-7 and HeLa cancer cells indicated the effective localization of BTPP and BeTPP within cancer-cell mitochondria. Under light irradiation, BTPP and BeTPP exhibited robust photo-induced therapeutic effects in both cell lines, with half-maximal inhibitory concentration (IC50) values of ~30 and ~55 nM, respectively.

Poster Presentation : **PHYS.P-133**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Effect of vitamin C, B3 and E mixtures with fat-soluble vitamins on MMP-9 expression level

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Jaewon Choi and Namdoo KimDepartment of Chemistry, Kongju National University, Kongju 32588, Republic of KoreaMMP-9 is a zinc(II)-containing matrix metalloproteinase that plays critical roles in pathological process of various diseases such as Alzheimer’s disease, cardiovascular diseases, dry eye, arthritis, and cancer. It has been reported that cellular level of this enzyme is higher in tumor cells than normal cells. MMP-9 facilitates metastasis and progression of cancer due to its own function on extracellular matrix. It degrades type IV and V collagens and other extracellular matrix proteins. Our previous research states how fat-soluble vitamins affect the expression and enzymatic activity of MMP-2 and MMP-9. Here, we present how the combination of vitamin C, B3 and E with each fat-soluble vitamins (A, D and K) affect MMP-9 expression level and enzymatic activity. Cells were treated with vitamin mixtures at different doses for 24 hr after transfection. Fixation followed by immunostaining enabled us to label MMP-9 for fluorescence imaging. Acquired fluorescence images were analyzed to assess cellular expression levels.

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Poster Presentation : **PHYS.P-134**

Physical Chemistry

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CO_2 Laser-induced $CoFe_2O_4$@NC hollow cubes from CoFe-Prussian Blue Analogues for Electrochemical Nitrate Reduction

Yeryeong Lee, Theerthagiri Jayaraman, Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

Nitrogen pollution stemming from the excessive use of nitrogen fertilizers and industrial emissions has become a serious environmental concern. Various technologies exist for mitigating nitrate contamination, with the electrochemical method standing out due to its high treatment efficiency, relatively low investment cost, and lack of reliance on external chemical modification. Nevertheless, the electrochemical nitrate reduction reaction (NO_3^-RR) is intricate and may yield diverse products. Therefore, efficient and selective removal of nitrate is essential.In this study, hollow particles of CoFePBA were synthesized, maintaining their structure through the use of a CO_2 laser, and subsequently employed in the NO_3^-RR reaction. The synthesized materials underwent comprehensive characterization using techniques such as scanning electron microscopy (SEM), Raman spectroscopy, X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM). These analyses confirmed the successful synthesis and offered valuable insights into the structural and compositional properties of the materials. The electrocatalytic activity of the synthesized material was assessed by measuring the LSV efficiency under alkaline conditions. In the NO_3^-RR, NO_3^- undergoes reduction to form various intermediates. The concentrations of NO_3^-, NH_3, and NO_2^- were measured using UV-Vis spectroscopy to evaluate the performance of NO_3^-RR. In summary, this study aims to evaluate the efficiency of NO_3^-RR and subsequently apply it to an environmentally friendly zinc nitrate battery system with high energy density. Such a system could serve as a renewable energy storage solution, contributing to the development of eco-friendly processes and enhancing energy production efficiency.

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Physical Chemistry

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Investigation of Trap State Suppression in Mg-Doped CsPbBr3 Perovskite Quantum Dots at the Single Particle Level

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The presence of localized trap states on the surface of cesium lead halide (CsPbX3) perovskite quantum dots (PQDs) is one of the greatest obstacles to the commercialization of perovskite-based optoelectronic and photovoltaic devices. Surface passivation by post-synthetic metal halide treatment is considered a promising strategy to suppress surface defects in inorganic lead halide perovskites and elevate the efficiency of devices based on these materials. Herein, we synthesize CsPbBr3 PQDs by ligand-assisted reprecipitation (LARP) method and develop a facile ambient post-synthetic MgBr2 treatment protocol. Through MgBr2 doping, we measure narrower full width at half maximum (FWHM), and higher photoluminescence quantum yield (PLQY) than pristine CsPbBr3 PQDs. We investigate PL blinking at a single particle level using a home-built laser scanning confocal fluorescence microscope to elucidate the degree of defects changed by doping and the correlation between trap states and charge carrier recombination. As a result of doping, Mg-doped CsPbBr3 PQDs show improved PL lifetimes (τ) and longer duration of ON-states (τ_ON), indicating the effective suppression of surface traps. Our experimental results provide an insightful understanding of the passivating roles of MgBr2 on the surface of CsPbBr3 PQDs.

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Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

In Situ Growth of NiFe Layered Double Hydroxide on Nickel Foam via Pulsed Laser for Oxygen Evolution Reaction

Dong Hyeon Lee, Chae Eun Park, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

In this study, we developed a new method for fabricating binder-free electrode materials using the pulsed laser irradiation (PLI) technique. The laser beam was directed onto the surface of nickel foam (NF), causing the NF to oxidize and transform into nickel hydroxide ($Ni(OH)_2$). By employing microwaves, it became possible to form NiFe layered double hydroxide (LDH), a compound challenging to produce through laser irradiation alone, on the NF surface. The synthesized materials underwent characterization using XRD, Raman, FE-SEM, and XPS analytical techniques and were utilized for the oxygen evolution reaction (OER) in 1.0 M KOH. NiFe LDH exhibited superior activity compared to pure NF in the OER. Furthermore, the electrocatalytic activity of NiFe LDH will be tuned by converting it into NiFeP through a phosphidation process.

Poster Presentation : **PHYS.P-137**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Laser-Assisted Synthesis of $BaTiO_3$/MXene Composites for Enhanced Supercapacitor Performance

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The integration of advanced materials in supercapacitor design has significant attention due to their potential to address the ever-increasing demand for high-performance energy storage devices. In the present work we report the laser-assisted synthesis of $BaTiO_3$/MXene nanocomposites tailored for superior supercapacitor applications. The incorporation of MXene into the $BaTiO_3$ framework has shown significant enhancements in specific capacity and long-term stability. Structural and morphological analyses revealed particle sizes within the range of 80-100 nm, indicative of the successful synthesis of nanocomposite materials. Galvanostatic charge-discharge (GCD) analyses further demonstrated the superior performance of the $BaTiO_3$/MXene supercapacitors, exhibiting enhanced specific capacity compared to pure $BaTiO_3$ counterparts. Moreover, the stability of these supercapacitors over long life cycles shows their potential for practical energy storage applications. Moreover, the $BaTiO_3$/MXene composite exhibited excellent stability over long cycling life, making it a promising candidate for high-performance supercapacitor applications.

Poster Presentation : **PHYS.P-138**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Stabilization of iridium on N-doped porous carbon to boost electrocatalytic overall water splitting

Seong Bo Lee, Maheskumar Velusamy, Ahreum Min, Cheol Joo Moon, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Electrochemical water splitting presents a significant approach to sustainable hydrogen energy production. However, the creation of dual-functional electrocatalysts with high activity and durability poses a critical challenge for alkaline overall water splitting. In this work, we propose a rapid and novel method for synthesizing a vastly efficient electrocatalyst: Zeolitic imidazolate framework (ZIF-8) derived N-doped porous carbon decorated with Ir catalyst (NC-Ir). The NC-Ir catalyst benefits from enhanced mass and charge transport through its ordered polyhedron carbon structure and exhibits strong metal-support interaction between Ir catalyst and the N-doped carbon framework. As a result, the NC-Ir catalyst reveals outstanding activity for both Hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) in alkaline electrolyte medium. The optimized NC-Ir catalyst showed excellent catalytic HER and OER performance with low overpotential, comparable to commercial Pt/C and IrO_2 catalyst, along with amazing catalytic stability for 12 h. Remarkably, overall water splitting system assembled with NC-Ir||NC-Ir as the cathode and anode, exhibits superior performance towards alkaline electrolysis with a low cell voltage and brilliant long-term stability. This work delivers a rapid and simple strategy for synthesizing bifunctional electrocatalyst suitable for cost-effective hydrogen production.

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Physical Chemistry

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Laser-induced Flowers-Like CuCo-Sulfides from Bimetallic CuCo Prussian Blue Analogues for Enhanced CO_2 Reduction Catalysis

<u>Juhyeon Park</u>, Ahreum Min, Cheol Joo Moon, Theerthagiri Jayaraman, Soohan Yun, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Examining the catalyst formation mechanism and producing precisely controlled catalysts are indispensable aspects of materials and catalytic chemistry. In this study, flower-shaped CuCo sulfides were synthesized using bimetallic CuCo Prussian blue analogs (PBA) via pulse laser irradiation (PLI) process. Real-time confirmation of sulfide formation by PLI was achieved through Raman spectroscopy using an acoustic resonance device. The catalytic potential of these sulfides in the CO_2 reduction reaction was demonstrated. Initially, sulfur decomposed by the laser combined with the CN groups of PBA to form thiocyanate, followed by rapid reactions with copper to produce Cu_2S and subsequent reactions with cobalt to form Co_9S_8. Moreover, the correlation between the sulfide shapes and laser parameters was observed, indicating the influence of laser parameters on the formation mechanism. Additionally, well-defined and tunable CuCo sulfides exhibited remarkable results in selectively reducing carbon dioxide to produce acetone. This study contributes to enhancing the selectivity of controlled catalyst synthesis and providing efficient electrocatalysts for CO_2 Reduction.

Poster Presentation : **PHYS.P-140**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Directional Electron Transfer Across Semiconductor based materials - Embedded Photocatalytic Membrane

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Photocatalyst membranes prepared with semiconductor nanoparticles embedded in polymer film offer a convenient approach to direct the electron and hole flow and separate reduction and oxidation products. We have now embedded In2S3 and ZnS semiconductor nanoparticles in a Nafion membrane to induce photocatalytic reactions using visible light. In addition, we have incorporated a viologen redox relay within the membrane to facilitate electron transfer to thionine (TH) dissolved in water. By inserting the photocatalytic membrane in an H-cell, we can separate the oxidation and reduction products and track the electron flow using steady state photolysis and transient absorption spectroscopy. The enhanced charge separation in In2S3 and ZnS heterostructure at 50:50 loading allowed us to maximize the electron transfer yield. Directing such vectorial charge transfer in a photocatalytic membrane will be useful in suppressing undesired side reactions (e.g. reoxidation of a reduced product) and facilitating product separation.

Poster Presentation : **PHYS.P-141**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Exploring the Impact of Pd Nanoparticles on $NiCo_2O_4$ Electrocatalyst for Enhanced Hydrazine-Assisted Hydrogen Production

Senthil Raja Arumugam, Sieon Jung, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Recent attention has been focused on hybrid water electrolysis utilizing the hydrazine oxidation reaction (HzOR) instead of the slower anodic oxygen evolution reaction (OER) for efficient hydrogen production. The development of highly effective bifunctional electrocatalysts capable of catalyzing both the hydrogen evolution reaction (HER) and HzOR is crucial for fabricating cost-effective hybrid water electrolysis systems. In this study, we designed and synthesized Pd nanoparticles decorated on $NiCo_2O_4$ nanoplates to serve as a bifunctional electrocatalyst for both HER and HzOR. The synthesis process involved the production of $NiCo_2O_4$ nanoplates through a combination of hydrothermal reaction and high-temperature calcination. Subsequently, Pd nanoparticles were decorated onto the $NiCo_2O_4$ nanoplates using pulsed laser irradiation (PLI) to create the $Pd/NiCo_2O_4$ composite. The optimized $Pd/NiCo_2O_4$ composite exhibited outstanding electrocatalytic performance, demonstrating a low overpotential of 294 mV for HER and an ultra-small working potential of –6 mV (vs. RHE) for HzOR at 10 mA cm^{-2} in a 1 M KOH electrolyte. Consequently, an overall hydrazine splitting (OHzS) electrolyzer employing the $Pd/NiCo_2O_4 \parallel Pd/NiCo_2O_4$ system consumed low cell voltages of 0.35 V and 0.94 V to supply current densities of 10 mA cm^{-2} and 100 mA cm^{-2}, respectively. This study presents a facile strategy for engineering bifunctional electrocatalysts suitable for energy-efficient hydrogen production

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Physical Chemistry

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Pulsed Laser Synthesis of CuO@Co Nanorods as Efficient Electrocatalyst for Oxygen Evolution Reaction

Jangyun Kim, Chae Eun Park, Theerthagiri Jayaraman, Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

Rod-shaped nanoparticles exhibit a higher surface-to-volume ratio compared to spherical particles, leading to increased chemical reactions or interactions on the particle's surface. Consequently, they demonstrate elevated activity when employed as electrochemical catalysts. In this study, nanorod-shaped CuO@Co alloy was synthesized via pulsed laser ablation (PLA) in methanol. The intrinsic physicochemical properties of the CuO@Co nanorods catalysts were confirmed through UV-Vis, Raman spectroscopy, X-ray diffractometry (XRD), and field emission scanning electron microscopy (FE-SEM). Furthermore, electrochemical analyses revealed the superior catalytic performance of CuO@Co nanorods in oxygen evolution reaction. The unique morphology and composition of the nanorods contribute to their enhanced activity, making them promising candidates for efficient electrocatalysis. The findings of this study provide valuable insights into the design and application of rod-shaped nanoparticles for advanced electrochemical systems.

Poster Presentation : **PHYS.P-143**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Anion exchange in highly luminescent lead free halide perovskites ($CsCuX_3$, X= Br, Cl)

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The present study investigates post-synthesis chemical transformations of colloidal nanocrystals, focusing on anion-exchange reactions in lead-free cesium halide perovskite nanocrystals. While cation-exchange is commonly employed, anion-exchange reactions in lead-free halides remain relatively unexplored. The novelty of lead-free cesium halide perovskite nanocrystals, with a crystal structure compatible with existing cesium lead halides, has garnered significant interest. The current work presents a pioneering approach to tunable anion exchange in $CsCuBr_3$ nanocrystals to form $CsCuCl_3$ perovskite. Anion exchange extents are monitored through shifts in fluorescence emission peaks and ultraviolet-visible absorbance edges, controlled by adjusting absorbed doses. The study reports fast, room temperature, and deliberately partial or complete anion-exchange in luminescent semiconductor nanocrystals of lead-free cesium halide perovskites ($CsCuX_3$, X = Cl, Br, I). Tuning the halide ratios enables the precise adjustment of photoluminescence across the entire visible spectral region (410–510 nm) while maintaining high luminescence and broad emission in the blue-green region. Additionally, the study demonstrates fast anion-exchange, resulting in uniform $CsCu(Cl/Br)_3$ in appropriate ratios.

Poster Presentation : **PHYS.P-144**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Unveiling the Superior Electrocatalytic Role of Multicomponent High-Entropy Alloys in Nitrite Reduction Reaction

Sieon Jung, Senthil Raja Arumugam, Heeeun Ahn[1], Wonji Go[1], Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

[1]*Department of chemistry, Gyeongsang National University, Korea*

Electrochemical nitrite reduction presents a sustainable and efficient alternative to the Haber–Bosch process for ammonia production, offering reduced energy consumption and minimal CO_2 emissions at ambient conditions. However, challenges persist in achieving electrocatalysts with high efficiency and selectivity. In this study, we synthesized low-to-high entropy alloys using pulsed laser techniques. The innovative pulsed laser technology allowed for the synthesis of alloys spanning from low entropy to high entropy by adjusting the number of elements involved. High entropy alloys (HEAs) demonstrate exceptional performance in the nitrite reduction reaction (NO_2RR) owing to their diverse active sites and structural flexibility, which optimize interactions with reactants and enhance catalytic efficiency. In a 0.5 M Na_2SO_4 solution containing 200 ppm $NaNO_2$, the freestanding HEA electrode achieves a high faradaic efficiency (FE) of 86.75% at -0.6 V vs. RHE, with excellent stability. This study contributes to the design and development of efficient, stable electrocatalysts via laser technology for the electrocatalytic production of ammonia by removing nitrite waste from wastewater.

Poster Presentation : **PHYS.P-145**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pulsed-Laser Grown Nickel sulfo-selenide Nanostructures for Water and Furfural Electrooxidation Reactions

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Department of Chemistry, Gyeongsang National University, Korea

In this wok, we introduce a pulsed laser ablation in liquids (PLAL) approach for synthesizing dianionic sulfur-selenide fused nickel-chalcogenides ($Ni_3S_xSe_{4-x}$), facilitating electrochemical OER and furfural oxidation reaction (FOR) in alkaline media. Incorporating Se and S anions into $Ni_3S_xSe_{4-x}$ modulates the electronic structure of Ni, thereby enhancing its intrinsic electrocatalytic activity and stability for OER, achieving an overpotential of 326 mV at 10 mA/cm^2 and a Tafel slope of 214 mV/dec in 1.0 M KOH. Furthermore, FOR catalyzed over $Ni_3S_xSe_{4-x}$ produces approximately 13.7 mM furoic acid with a selectivity of ~73.14%, carbon balance of ~89.94%, and a notable Faradaic efficiency of approximately 98.82% over 2 h at 1.58 V vs. Reversible Hydrogen Electrode. This research underscores the effectiveness of the laser-patterned nickel sulfo-selenide in modulating oxidation activity, contributing significantly to the selective valorization of biomass.

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Poster Presentation : **PHYS.P-146**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pulsed Laser Synthesis of Carbon-Coated Ruthenium Nanoparticles for Hydrazine-Assisted Efficient Hydrogen Production

Heeeun Ahn, Senthil Raja Arumugam, Sieon Jung, Wonji Go[1], Myong Yong Choi[*]

Department of Chemistry, Gyeongsang National University, Korea

[1]*Department of chemistry, Gyeongsang National University, Korea*

Hydrazine oxidation reaction (HzOR) has been investigated as a potential alternative to the oxygen evolution reaction (OER) to increase the production efficiency of green hydrogen even at low voltage. However, developing efficient bifunctional electrocatalysts capable of catalyzing both the cathodic hydrogen evolution reaction (HER) and the anodic HzOR in hybrid water electrolysis remains challenging. In this study, we developed carbon-coated face-centered cubic (fcc) Ru nanoparticles using the pulsed laser ablation in liquid (PLAL) approach. The electrochemical results revealed that the optimized Ru@C catalyst exhibited a low potential of 61 mV at 10 mA cm^{-2} for the HER in a 1 M KOH solution. Additionally, it demonstrated a low working potential of -0.032 V at 10 mA cm^{-2} for the HzOR in a 1 M KOH/0.5 M hydrazine solution. This demonstrates the excellent bifunctional activity of Ru@C for both HER and HzOR, attributed to the highly catalytic active fcc Ru nanoparticles covered by the good conductive, large surface area, and highly stable carbon layers. As a result, the hydrazine splitting (OHzS) electrolyzer offers an energy-efficient approach for producing high-purity hydrogen. This study introduces a novel approach to synthesizing a highly effective Ru@C electrocatalyst for energy-efficient hydrogen production

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Physical Chemistry

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Full quantum electron transfer theory

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Electron transfer is essential in material science, electrochemistry, and biochemistry, underscoring the importance of an insight for the fundamental process. The Marcus theory is representative of the formulas used to describe electron transfer, yet current dynamics methods have struggled to accurately reproduce its prediction, mainly due to inadequate consideration of decoherence. We propose the Full Quantum Electron Transfer (FQET) theory, which not only analytically derives the golden rule rate, including Marcus rates, but also enables the execution of real-time electron transfer simulations. Through our two-state numerical simulations, we accurately replicate the predictions of Marcus theory and reveal the significant impact of quantum coherence on electron transfer. This effect is significant in conditions of lower reorganization energy and temperature, aligning with longer decoherence times. Additionally, our numerical simulations within the strong coupling regime, which beyond the golden rule limits, reveal deviations in the electron transfer process from Marcus theory, highlighting the FQET theory's potential to explore previously undiscovered electron transfer dynamics. Thus, FQET theory, by properly incorporating decoherence, both recovers the traditional electron transfer theory and provides a framework that enables the analysis of previously unexplored regimes of electron transfer.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **PHYS.P-148**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pulsed Laser Engineering of AgCu Electrocatalyst for Efficient Hydrogen Production via Formaldehyde Oxidation Reaction

Wonji Go, Senthil Raja Arumugam[1], Sieon Jung[2], Heeeun Ahn[3], Myong Yong Choi[1,*]

Department of chemistry, Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*
[2]*Gyeongsang National University, Korea*
[3]*Chemistry, Gyeongsang National University, Korea*

To address energy and environmental challenges, extensive research is underway on hydrogen energy as a renewable and clean high-energy source. Hydrogen energy production via overall water splitting (OWS) involves both the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER). The OER, with its high energy requirements, serves as a rate-determining step in OWS, prompting research efforts to explore alternative reactions. This study focuses on synthesizing the AgCu electrocatalyst via a facile and rapid pulsed laser approach to catalyze the formaldehyde oxidation reaction (FOR), aiming to mitigate the energy demands associated with the OER and enhance hydrogen energy production efficiency by facilitating hydrogen generation at both the anode and cathode. As expected, the electrochemical results show that the synthesized AgCu catalyst exhibited excellent electrocatalytic activity towards the FOR using a formaldehyde-contained 1 M KOH electrolyte. Specifically, the integration of HER and FOR in an electrolyzer not only offered efficient hydrogen production but also co-synthesized formic acid, both at a low voltage. This study presents an effective strategy for developing potential electrocatalysts for large-scale hydrogen production

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Poster Presentation : **PHYS.P-149**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Boosting Rate Capability and Energy Density of Nickel Cobalt Oxalate / MXene Composite Based Supercapacitors

Hansu Kim, Anil Kumar Astakala, Yiseul Yu, Seung Jun Lee*

Department of IT-Energy Convergence (BK21 FOUR), Korea National University of Transportation, Korea

Energy storage technologies play a pivotal role in addressing the increasing demand for efficient and sustainable energy applications. In the present work, we report a comprehensive electrochemical characterization of Ti_3C_2 MXene interfaced nickel cobalt oxalate (MX/NCO) composite for energy storage in supercapacitors. The synthesized NCO and MX/NCO composite materials formation is confirmed by XRD and Raman analysis. The synthesized MX/NCO composite was used as active material along with PVDF binder and carbon black as a conductive additive for the preparation of electrodes to fabricate a symmetric supercapacitor. The electrochemical characterization of the fabricated supercapacitors was investigated through cyclic voltammetry (CV), electrochemical impedance spectroscopy, and charging-discharging studies. The MX/NCO composite electrodes performed superior cycle life and specific capacitance than the pristine NCO and MXene. The electrochemical superiority of the MX/NCO composite was attributed to the synergistic effects arising from the combination of Ti_3C_2 MXene with excellent conductivity, large surface area, and the redox activity of NCO. The present research contributes significantly to the development of advanced energy storage systems, offering insights into the design and optimization of supercapacitors with tailored electrode materials and interfaces.

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Poster Presentation : **PHYS.P-150**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Ru-doped NiCo Layered Double Hydroxide via Pulsed Laser Rotating System

<u>Soohan Yun</u>, Ahreum Min, Cheol Joo Moon, Juhyeon Park, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Two-dimensional Layered Double Hydroxides (LDHs) have garnered attention as crucial electrode materials owing to their high activity, tunable composition, and unique structure. However, conventional synthesis processes involve high heat and extended durations. In this study, we eco-friendly synthesized NiCo LDH rapidly using a pulsed laser rotating system. The morphology and composition of the resulting LDH were determined through SEM and SEM-EDS analysis, while structural features were studied via XRD and Raman spectroscopy. To enhance electrochemical efficiency, our future work involves doping Ru using a pulsed laser rotating system, followed by conducting electrochemical water splitting experiments.

Poster Presentation : **PHYS.P-151**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Designing a MXene/Carbon Nitride Hybrid Material to Enhance the Stability of High-Energy Lithium-Ion Batteries.

Young Soo Kim, Anil Kumar Astakala, Yiseul Yu, Seung Jun Lee*

Department of IT-Energy Convergence (BK21 FOUR), Korea National University of Transportation, Korea

In response to the escalating demand for energy storage solutions, the current era witnesses continuous growth and innovation. Lithium-Sulfur batteries (LSBs) emerge as promising post-Lithium era storage devices, boasting six times the capacity of traditional Lithium-ion batteries. However, LSBs encounter challenges, primarily the shuttle effect, hindering their performance. This study focuses on addressing these challenges by investigating the potential application of a sulfur and carbon (S/C) composite in LSBs. The synthesis of a CxNy phase through hydrothermal methods, confirmed via XRD analysis, contributes to this endeavor. The optical absorption spectra of the synthesized CxNy exhibit strong absorption in the visible region, indicating its potential effectiveness. By incorporating CxNy and MXene into the composite, efforts are made to mitigate the shuttle effect and enhance electron conductivity. Furthermore, employing 1M LiTFSI in DME:DOL as the electrolyte enhances the overall performance. Electrochemical analysis techniques, including cyclic voltammetry, electrochemical impedance spectroscopy, and galvanometric charge-discharge studies, are utilized to evaluate the assembled LSBs. Results demonstrate significantly enhanced electrochemical performance, characterized by good specific capacity retention even after harsh C-rate analysis and improved cycling stability. This research represents a substantial contribution to advancing energy storage systems, offering valuable insights into the design and optimization of supercapacitors through tailored electrode materials and interfaces.

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Poster Presentation : **PHYS.P-152**

Physical Chemistry

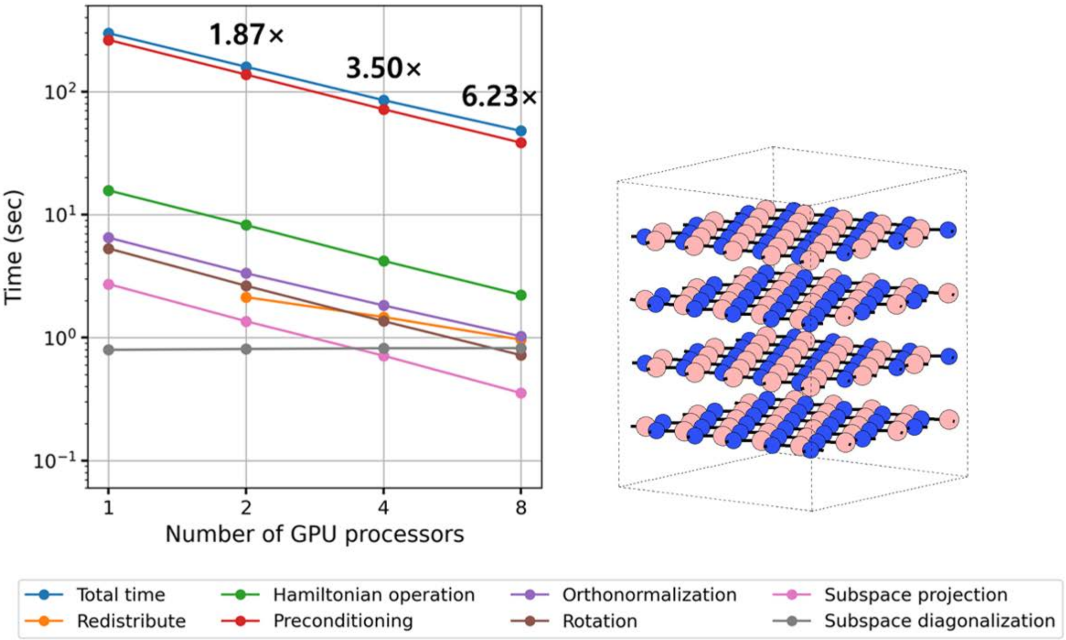
Exhibition Hall 2 THU 11:00~13:00

Development of Efficient Eigenvalue Solver for Multi-GPU Accelerated Density Functional Theory Calculations

Jeheon Woo, Woo youn Kim*

Department of Chemistry, KAIST, Korea

In pursuit of accelerating the iterative diagonalization of electronic structure calculations, this study presents an enhanced modification to the shift-and-invert preconditioning method.Our approach involves correcting the Ritz value shifts utilizing the residuals to be closer to the exact eigenvalues, which leads to a significant increase in the convergence speed of the iterative diagonalization.Furthermore, we achieve rapid evaluation of the shift-and-invert preconditioning through an efficient implementation of the preconditioned conjugate gradient solver.Leveraging state-of-the-art GPUs, we validate the effectiveness of our method on real-space density functional theory (DFT) calculations of 1D, 2D, and 3D periodic systems.Our method attains both fast diagonalization and high multi-GPU parallel efficiency, completing the self-consistent field calculation of systems with hundreds of atoms in approximately 10 seconds on a single GPU node.As a result, this study contributes to the overarching objective of enhancing the efficiency of electronic structure calculations.


1.87×
3.50×
6.23×
Time (sec)
10^2
10^1
10^0
10^{-1}
1
2
4
8
Number of GPU processors
Total time
Redistribute
Hamiltonian operation
Preconditioning
Orthonormalization
Rotation
Subspace projection
Subspace diagonalization

Poster Presentation : **PHYS.P-153**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Low-Voltage-Driven Dual Hydrogen Production with Value-Added Formate Co-synthesis on Laser-Developed Ru/Cu Electrocatalyst

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Department of Chemistry, Gyeongsang National University, Korea

Due to the slow kinetics and high overpotential required, there is a pressing need to find more thermodynamically favorable reactions for water electrolysis than the oxygen evolution reaction (OER). Recently, there has been considerable interest in the partial oxidation of formaldehyde to produce hydrogen gas and formate at anode under alkaline conditions as a potential alternative to the OER. Therefore, in this study, we present a straightforward approach for designing and synthesizing Ru/Cu composites as bifunctional electrocatalysts for both the hydrogen evolution reaction (HER) and formaldehyde oxidation reaction (FOR). To achieve this, Ru-doped CuO microplates were initially synthesized using a coprecipitation method, which were then transformed into spherical-shaped Ru/Cu composites via facile pulsed laser irradiation in liquid (PLIL) method. The optimized 0.2Ru/Cu composite exhibited a low overpotential of 182 mV (vs. RHE) at 10 mA cm^{-2} for the HER in a 1 M KOH electrolyte and an ultra-low working potential of –0.078 mV (vs. RHE) for FOR at 10 mA cm^{-2} in a 0.6 M HCHO solution in 1 M KOH electrolyte. This confirms its bifunctionality in the FOR-coupled water splitting (FOR||HER) electrolyzer. As a result, the assembled 0.2Ru/Cu || 0.2Ru/Cu system required low cell voltages of 0.43 and 0.86 V to achieve current densities of 10 and 40 mA cm^{-2}, respectively. Therefore, the synthesized 0.2Ru/Cu composite shows great promise as a material for efficient hydrogen production from both cathode and anode with value-added formate co-synthesis at a low voltage.

Poster Presentation : **PHYS.P-154**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Coordination Chemistry of Semi-constrained Systems: DFT Study

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

Metal complexes with constrained or semi-constrained geometry play a crucial role in the coordination chemistry of the metalloenzymes by imposing structural limits on the ligands. Metal substitution of a metalloenzyme significantly alters the geometry of the active site due to differences in coordination preferences, sizes, and electronic configurations. In this work, we selected the catalytic active centre of carbonic anhydrase (CA), a metalloenzyme, and its four metal variants containing Co^{2+}, Ni^{2+}, Cu^{2+}, and Zn^{2+} as the model system and conducted a density functional theory (DFT) study on their coordination chemistry. As the structures of these metal variants have already been reported experimentally, we utilized various functional and basis set combinations to find the optimal combination that reproduces the experimental structures and found that M06-2x functional with 6-311++G(d,p) basis set with LANL2DZ effective core potential is suitable for our model system. Interestingly, we found that the native metal ion in metalloenzyme does not always have the strongest binding, and metal substitution adheres to the Irving-William series. Metal ions in high- and low-spin states prefer a particular geometry, even in a semi-constraint environment. Our findings can be utilized to design and tune the geometry around a metal ion in various semi-constraint systems, like the active site of an artificial metalloenzyme.

Poster Presentation : **PHYS.P-155**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Degradation of dyes according to surface charge of photocatalyst and enhancement of catalytic activity by nanoparticle clusters

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Synthetic dyes are used across industries such as food, textiles, cosmetics, and paints due to their advantages such as stability and wide application, but such wastewater causes environmental pollution and genotoxicity in humans. The chromophore and auxochrome that make up the dye contribute to improving the color development ability and dye solubility of synthetic fibers and substances with various properties, and depending on the characteristics of the functional group, they exhibit different interactions with the catalyst and affect the degradation of dyes. In this study, we use plasmonic photocatalysts, Au nanoparticles (Au NPs) and Au nanoparticle clusters (Au NPCs), using light energy in the visible light region to explore degradation mechanisms caused by interactions between photocatalysts and various type of dye molecules. Light-induced localized surface plasmon resonance (LSPR) of Au NPs can decompose photostable synthetic dyes. The hot spot generated by interaction within the interparticle gap of Au NPCs, which is an assembly of nanoparticles, has a higher degradation efficiency than that of a single nanoparticle, and photocatalytic activity increases as the intensity of light increases. We experiment dyes degradation under LED solar simulator illumination and analyse with UV-vis spectrophotometer. These study provide valuable insight into the interaction of catalysts with molecules targeted for degradation through the synthesis of cluster-shaped nanoparticles rather than controlling parameters such as size or shape of the nanoparticles (rod, sphere, cube, etc.). As a result, it could lead to interesting research of degradaion mechanism to dyes according to the interaction between catalysts and molecules.

Poster Presentation : **PHYS.P-156**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Exploring the bifunctionality nature of Ir doped CoGa-LDH synthesized via laser irradiation system towards overall electrochemical water-splitting

Akash Prabhu Sundar Rajan, Theerthagiri Jayaraman, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

A new class of two-dimensional materials known as layered double-hydroxides (LDHs) has emerged as promising candidates for various applications, owing to their unique features such as well-defined morphology, large specific surface area, and cation-exchange ability. Herein, we report the successful synthesis of iridium-doped cobalt-gallium-LDH (Ir-CoGa-LDH) using a one-pot pulsed laser irradiation (PLI) strategy. The synthesized materials were characterized using SEM, Raman spectroscopy, XRD, and XPS, which confirmed the successful synthesis and provided insights into their structural and compositional properties. Subsequently, the electrochemical activity of synthesized Ir-CoGa-LDH was evaluated for both the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in an alkaline medium. Remarkably, the Ir-CoGa-LDH sheets exhibited significantly enhanced activity with low overpotential of 204 mV @ 10 mA cm^{-2} for HER compared to CoGa-LDH (336 mV). Likewise, for OER, the Ir-CoGa-LDH sheets displayed significantly enhanced activity with a low overpotential of 294 mV @ 10 mA cm^{-2} than that of CoGa-LDH (482 mV). Especially, the one-pot PLI approach used in the synthesis of Ir-CoGa-LDH demonstrated several unique characteristics, including rapid processing, cleanliness, the absence of additional surfactants or reducing agents, and no generation of byproducts during materials development. These results highlight the potential of Ir-CoGa-LDH as a highly efficient and environmentally friendly electrocatalyst for electrochemical hydrogen production.

Poster Presentation : **PHYS.P-157**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

MXene/La_2CoNiO_6 Double Perovskite Composites for Supercapacitor Applications

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Department of IT-Energy Convergence (BK21 Four), Korea National University of Transportation, Korea

In the quest of advancing energy storage technologies, the synergistic integration of two distinct materials has garnered significant attention. In current work, we report the synthesis and characterization of MXene/La_2CoNiO_6 double perovskite composites tailored for supercapacitor applications. MXenes, known for their exceptional conductivity and high surface area, were synthesized and KOH assisted La_2CoNiO_6 double perovskite nanoparticles were prepared using a simple wet chemical method. The composite materials were then fabricated through a simple mixing and subsequent annealing process. The structural, morphological, and electrochemical properties of the composites were thoroughly investigated. X-ray diffraction (XRD) and scanning electron microscopy (SEM) confirmed the successful formation of the composites with a well-defined structure and intimate interfacial contact between the components. Electrochemical characterization revealed superior capacitance and cycling stability of the MXene/La_2CoNiO_6 composites compared to individual components, attributed to the synergistic effects arising from the combination of MXenes high conductivity and La_2CoNiO_6 pseudocapacitive behavior. Furthermore, the composites exhibited better rate capability, making them promising candidates for high-performance supercapacitor applications. The synergistic effect between MXene and La_2CoNiO_6 components in the composite structure contributes to enhanced electrochemical performance, making these composites promising candidates for high-performance supercapacitor applications.

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Poster Presentation : **PHYS.P-158**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Applications of Alchemical Free Energy Methods in Protein Interactions

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Department of Chemistry, Pusan National University, Korea

Since the emergence of computational methodologies such as molecular dynamics (MD) simulations, the simulation methods have been serving as a complementary tool for wet-lab experiments. In recent years, MD simulations have been increasingly incorporated into various research fields, with protein and drug research benefiting substantially. One of the most utilized methods among the computational investigations is alchemical free energy methods, which enable the prediction of binding affinities between proteins and small molecules. Here we suggest two applications of alchemical free energy methods across diverse protein systems.The first topic is the computational investigation of the thermodynamic stability of an oxygen molecule within the maltose-binding protein (MBP). MBP is a metabolic enzyme responsible for the utilization of maltose and maltodextrins. A recent experiment revealed that MBP can serve as a scaffold that contributes to the generation of reactive oxygen species, resulting in the intracellular accumulation of oxidative stress. We conducted free energy calculations on the MBP-O_2 complex and found out that the binding free energy difference between MBP and the O_2 molecule was negligible, within the thermal energy at room temperature.Secondly, we applied the alchemical methods to engineer the binding affinity of green fluorescent protein (GFP) through single-point mutations. GFP has been used as one of the most effective agents for fluorescence microscopy, and it exhibits weak homodimerization at high concentrations. We utilized a machine-learning method and the alchemical approaches to systematically mutate the interface of GFP homodimers and predict the binding affinity change upon each mutation. The results demonstrated that both the machine-learning method and the MD simulations had an overall correlation in predicting binding affinities of GFP.We expect our study to broaden the applications in the calculation of binding energies according to various protein

interactions. Specifically, our methods can be applied to the optimization of lead compounds in drug discovery and the prediction of the effects of disease-induced mutations in protein folding and binding.

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Poster Presentation : **PHYS.P-159**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pulsed laser decorated Pt nanoclusters on N-doped mesoporous carbon as robust electrocatalyst for hydrogen production via natural seawater splitting

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Department of Chemistry, Gyeongsang National University, India

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

Seawater electrolysis presents an attractive alternative to conventional freshwater electrolysis for hydrogen production, exploiting on the vast availability of this resource on Earth. However, the development of efficient electrocatalysts for the hydrogen evolution reaction (HER) in alkaline seawater remains a critical challenge. In this work, we present a novel and advanced method for fabricating a highly efficient electrocatalyst: nitrogen-doped porous carbon decorated with platinum nanoclusters (NC-Pt), derived from metal-organic framework (ZIF-8). The as-synthesized NC-Pt catalyst produced numerous benefits, including a large surface area, porous structure, superior conductivity, N rich carbon, abundance of active metal sites, low Pt nanoclusters, while most importantly, strong interaction between NC matrix and Pt metal. These properties promote efficient mass transport during the HER process, resulting in significant enhancement in intrinsic performance. Consequently, the NC-Pt catalyst exhibits outstanding performance in both alkaline and seawater electrolytes, comparable to commercial Pt/C catalysts. Particularly, the optimized NC-Pt-4 catalyst demonstrates excellent HER catalytic activity with minimal overpotential (52 and 57 mV) in alkaline and seawater electrolytes, respectively, at a current density of 10 mA cm^{-2}, while maintaining remarkable stability over 12 h. Notably, seawater electrolysis requires a slightly higher cell voltage (1.65 V) compared to freshwater electrolysis (1.60 V) at 10 mA cm^{-2}. Moreover, the NC-Pt catalyst exhibits exceptional long-term stability without noticeable performance degradation. This research study provides an efficient and quick method for fabricating cost effective and extremely effective electrocatalysts for hydrogen production from in both alkaline and alkaline seawater

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Poster Presentation : **PHYS.P-160**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Development of a protein-ligand 3D structure database for AI-based binding site prediction

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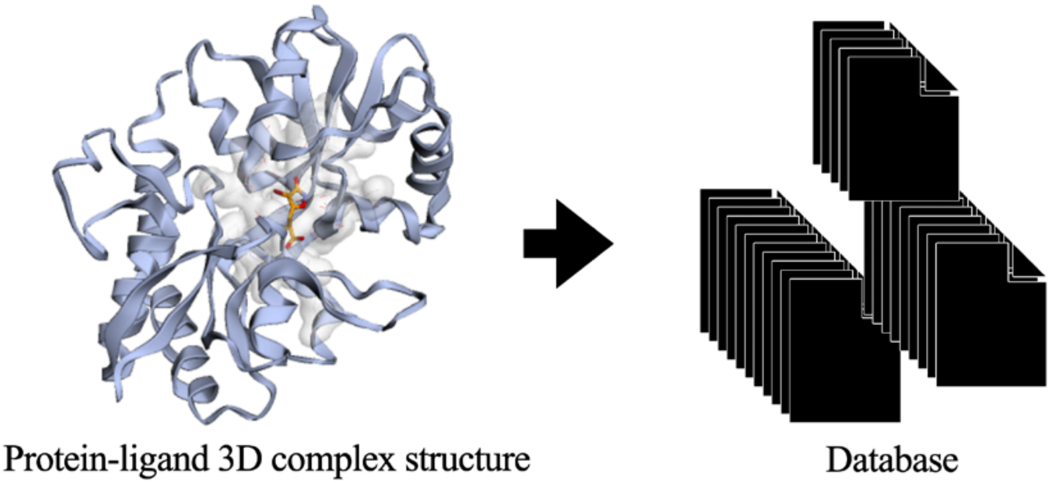
College of Pharmacy, Seoul National University, Korea
[1] *College of Pharmacy, Seoul National University, Korea*

Predicting binding sites is crucial in drug development, and AI models are increasingly becoming indispensable tools in this field. However, developing effective models necessitates access to high-quality, three-dimensional structured data. There is a recognized need for more contemporary and reliable data sources as many of the databases widely used in current research lack recent updates and improvements, highlighting a pressing need to meet the advanced requirements of modern research.We aim to develop a new database designed to improve the accuracy of binding site prediction models and to stay relevant to contemporary research needs. It is constructed based on the most recent data from RCSB PDB. Our methodology incorporates proven methods and employs distinctive strategies to preserve the uniqueness of the data. To ensure sustained relevance and utility, we plan to perform consistent updates to our database every two months.Our dataset provides a diverse range of binding site data, including not only small molecule ligands but also peptide ligands and metal cofactors. For user convenience and improved data utility, we offer sequence-based binding site labels and atom-level binding pockets in PDB format.We hope that our database will be a valuable resource for the advancement of binding site prediction, supplying high-quality data that can support researchers in creating accurate and dependable prediction models, and fostering progress in drug development.


Protein-ligand 3D complex structure
Database

Poster Presentation : **PHYS.P-161**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Elucidation of Equilibrium Size Distribution of Rigid Clusters and Liquid-like Droplets

Jingyu Kang, Jonghwa Han[1], Sangwoon Yoon[1], Sung Jee Kim[2], Ji-Hyun Kim[1,*], Jaeyoung Sung[1,*]

Chung-Ang University, Korea

[1]*Department of Chemistry, Chung-Ang University, Korea*

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

Supersaturation and nucleus seed formation are universal processes that precede all phase transitions. Despite extensive research on nucleation, our understanding on supersaturation, and nucleus seed formation remains rudimentary. In this poster, we present the exact statistical thermodynamic formula for the saturation degree, the most-probable size distribution of mesoscopic nuclei, and their phase transition, introducing the mesoscopic state defined by temperature, the total monomer concentration, and the largest cluster size (LCS). These results show that supersaturation emerges even at equilibrium for mesoscopic nuclei systems and decreases with the LCS. The size-distribution of nucleus seeds is either a unimodal or a monotonically decreasing function of size, depending on the system and temperature. There exists a critical supersaturation condition under which nucleus seeds undergo a phase transition, during which the most probable size exhibits an abrupt change. In addition, we found that our non-classical nucleation theory fit well in real systems; Gold Nanoparticle, FePt Nanoparticle, InP Quantum dot, mutant p53 aggregate, and IDP-2Yx2A micelle. This work can be extended to investigate diverse nucleation and phase transition phenomena prevalent across nature and industry.

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Poster Presentation : **PHYS.P-162**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

A Study of Surface on Aluminum Foils as an Anode in Various Electrolyte Concentration of Aluminum-ion Battery

Nattha Chaiyapo, Myong Yong Choi[1,*]

Department of Physics, Khon Kaen University, Thailand
[1]*Department of Chemistry, Gyeongsang National University, Korea*

Aluminum is a reliable material for use as an anode in aluminum-ion batteries (AIBs) due to its sustainable cycle. However, there have been conflicting studies regarding dendrite growth on aluminum foil surfaces. This study aims to clarify this issue by examining the characterization of aluminum foils as an anode with varying molar ratios of $AlCl_3$:EMIC ionic liquid electrolyte for AIBs. The results showed that when aluminum foils were immersed in these electrolytes for a period of time, their surfaces exhibited damage to the natural oxide layer. A micro-size deposition occurred on the aluminum surfaces in basic conditions, which is different from acidic conditions. After electrolyte immersion and cycling, the chemical composition of the aluminum surface was found to have changed, as observed through X-ray spectroscopy. These findings support the electrochemical reaction of AIBs at different concentrations of electrolyte and contribute to our understanding of the aluminum anode material used in ionic liquid electrolyte for AIB.

Poster Presentation : **PHYS.P-163**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Control of Structural Order of Aromatic Thiolate Monolayers on Au(111) Using Displacement Techniques

Dongjin Seo, Yeon O Kim, Hongki Kim, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are ultrathin films of organic molecules that spontaneously adsorb onto a metal surface and form an ordered shape. The properties of metal substrates, such as conductivity, optical properties, and binding energy, can be modified by regulating the formation conditions of SAMs. Aromatic thiol SAMs can influence the reactivity of the tail groups and the ability of the tail groups to bond with other species due to the extended π system. Electron radiation-induced cross-linking also increases the mechanical and thermal stability of aromatic SAMs. The high stability of the cross-linked aromatic SAMs allows them to be used for nanolithography and for films on the nanoscale. In this study, we studied the structure and formation of biphenyl-4-thiol (BPT). BPT SAMs formed partially ordered domains in DMF, EtOH solvent in a previous study. We used the displacement method in this study to form two-dimensional ordering aromatic thiol SAMs. Cyclohexane thiol (CHT) SAMs were used as a precovered layer in previous studies. CHT SAMs have an axial and equatorial form of CHT, so it has large intermolecular distance. Ordered single CHT SAMs were formed at RT EtOH 1 mM solution for 24 h in previous studies. In this study, we formed BPT SAMs SAMs in EtOH and DMF 1 mM solution at RT for 1min, 5 min, 30 min, and 1 h to study the formation process. Subsequently, we used scanning tunneling microscopy (STM), cyclic voltammetry (CV), and X-ray photoelectron spectroscopy (XPS) to investigate prepared BPT SAMs.

Poster Presentation : **PHYS.P-164**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Effect of Wingtip and Alkyl Backbone on the Formation and Structural Order of Self-assembled Monolayers on Au(111) from N-Heterocyclic Derivatives

Yeon O Kim, **Dongjin Seo**[1], **Hongki Kim**[1], **Jaegeun Noh**[1,*]

Hanyang University, Korea

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

Self-assembled monolayers (SAMs) functionalized with gold have significant uses in surface protection, catalysis, microelectromechanical systems, and sensing. Several scholars looked into thiol-based SAMs in their earlier research. However, thiols have a number of well-known disadvantages, despite their extensive use. It has been observed that thiol-based surfaces deteriorate considerably in a range of circumstances, including ambient air, heat treatment, and UV radiation. These shortcomings led researchers to discover more reliable and replaceable SAMs for gold surfaces. N-heterocyclic carbene (NHC) SAMs have a number of advantages over thiol-based SAMs, such as enhanced resistance to pH fluctuations, oxidative resilience, and heat. In this study, we created single-component SAMs on Au(111) and compared three classes of NHC benzimidazoles, also called standard carbenes. We synthesized 1,3-diisopropyl-6-(pentyloxy)-1H-benzimidazolium iodide (C5-iPr-NHC-I) and 6-(pentyloxy)-1H-benzimidazolium iodide (C5-NHC-I). And 1,3-diisopropylbenzimidazolium bromide (DIBI) was bought from TCI. The substituents bonded to NHC molecules have a significant impact on the binding, mobility, stability, and surface characterization of benzimidazolium NHC SAMs. The recent study found that while R'-groups attached to the backbone alter the NHC's electronic structure and offer a modular binding site for targets, R-groups attached to the NHC nitrogen, also known as wingtips, have a significant impact on the NHC's binding and orientation to the surface. The purpose of this study is to show the importance of the wingtip and alkyl chain backbone on adsorption conditions.

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Poster Presentation : **PHYS.P-165**

Physical Chemistry

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Synthesis and Photocatalytic Performance of La/TiO_2/GO/Halloysite Nanocomposite for Photodegradation of Organic Dyes

Hongki Kim, Dongjin Seo, Yeon O Kim, Jaegeun Noh[*]

Department of Chemistry, Hanyang University, Korea

Dealing with the challenge of wastewater purification is crucial in addressing environmental issues. This study introduces a new nanocomposite, La/TiO_2/GO/Halloysite, designed to improve the photocatalytic removal of pollutants like Rhodamine B. The unique tubular structure of halloysite, a naturally found aluminosilicate, makes it an excellent matrix for capturing contaminants. The pairing of titanium oxide (TiO_2) with La^{3+} ions reduces the band gap and enhances electron stimulation in TiO_2, producing a material with visible light photocatalytic properties. The incorporation of graphene oxide (GO) leads to further potential improvements in catalysis by facilitating more efficient electron movement. This could lead to a significant improvement in the degradation of organic compounds. In photocatalytic degradation of Rhodamine B by sunlight, the photodegradation efficiency of La/TiO_2/GO/Halloysite improved by 51% compared to La/TiO_2/Halloysite and 40% compared to TiO_2/GO/Halloysite. In order to thoroughly evaluate the prepared La/TiO_2/GO/halloysite nanocomposite, various analytical methods including XPS, XRD, FT-IR, BET, zeta potential measurement and SEM will be employed. The research objective is to illustrate the superior performance of the newly developed nanocomposite in eradicating organic dyes, thus contributing to the development of an effective, sustainable, and solar-powered wastewater purification solution.

Poster Presentation : **PHYS.P-166**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Observing energetic landscapes near the transition state in the frequency and time domain

<u>Junggil Kim</u>, Minseok Kang, Sang Kyu Kim[*]

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In this study, we have experimentally observed the energetic landscapes near the transition state of deuterated methylamine (CH3ND2) in the S1 state by employing the IR – UV double resonance spectroscopy in gas phase. Pre-excitation of the title molecule using the specific IR pulse wavelength prior to the S1 – S0 transition is found to allow the S1 population to access extremely highly-excited internal rotor states (up to m = 15) which is far beyond the adiabatic barrier height toward the N-D bond dissociation. In the frequency domain, it is expected by spectral analysis on the long progression of internal rotor states that severe structural changes in the N-D bond length should be accompanied as the total energy of the system gets closer to the top of the reaction barrier. In the time domain, S1 lifetimes directly measured from picosecond time-resolved pump-probe spectroscopy show an abrupt surge at ~ 1000 cm-1, indicating that the wavepacket localized in the potential well now possesses unbound character in that internal energy region. The unique spectral and dynamic patterns manifested in this study suggest that the internal rotation which is apparently perpendicular to N-D stretching motion is strongly coupled to the reaction coordinate in S1 CH3ND2, and also give deep insights into the topography of the adiabatic potential energy surface near the transition state. Semi-classical trajectory simulations based on a concept of classical path Hamiltonian nicely support our experimental findings.

Poster Presentation : **PHYS.P-167**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Light-driven electron dynamics of the Photoactive Yellow Protein derivatives

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Herein, we investigated the real-time dynamics of the first singlet electronic excited state (S_1) of deprotonated para-coumaric ester (pCE^-) and deprotonated para-coumaric acid (pCA^-) using nanosecond spectroscopy and femtosecond time-resolved spectroscopy combined with a cryogenically-cooled Paul ion trap. By measuring the S_1 lifetimes, we observed distinct relaxation dynamics for each derivative. In the case of pCE^-, the initial S_1 state bifurcates; one relaxation into the S_1 twisted intermediate, and the other undergoes an internal conversion (IC) to the Dipole-Bound state (DBS). Both of these bifurcated states subsequently undergoes autodetachment, resulting in the loss of an electron from the chromophore. However, in pCA^-, the initial S_1 state relaxes into an intermediate state characterized by a remarkably long lifetime. This intermediate state undergoes IC directly to the ground state (S_0), inhibiting autodetachment. We obtained evidence for this IC process by observing CO_2 fragmentation, indicating the generation of a hot S_0 state. The stark differences in the dynamics of the two derivatives can be attributed to the presence of the DBS. This suggests that the DBS, previously considered only as a 'doorway state', may also play a role in inhibiting the formation of anions. These findings provide valuable insights into the photoisomerization of the photoactive yellow protein.

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Poster Presentation : **PHYS.P-168**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Ultrafast Charge-Carrier Dynamics of the Green-Light Emitting InP/ZnSe/ZnS Core-shell Quantum Dots

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Investigation of photo-physical and photo-chemical properties of semiconductor materials could be achieved by the understanding of fundamental mechanisms in those materials. Most approaches for the characterization of semiconductor materials are focused in PL and EL (photo- and electro-luminescence) spectroscopy. However, it is worth to figure out in fs-ps dynamics of charge carriers due to the existence of non-radiative relaxation channels. Through various spectroscopic techniques with synchronized femtosecond (fs) and picosecond (ps) laser system, we study the charge carrier dynamics in InP/ZnSe/ZnS core-shell quantum dots.

Poster Presentation : **PHYS.P-169**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Layer-dependent exciton formation in two-dimensional crystals of perylene derivatives

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Organic crystals have garnered attention due to their flexibility, high strength, and their synthesis over large areas using diverse materials. Organic crystals can possess various types of excitons, with interactions occurring between them. In particular, two-dimensional organic crystals with a lower dielectric constant result in high exciton binding energies, making excitons crucial for the photophysical properties and applications of such crystals. Perylene derivatives, such as 3, 4, 9, 10-perylene tetracarboxylic dianhydride (PTCDA), are typical organic semiconductors with a layered structure and high carrier mobility. Although perylene derivatives' exciton formation process has been extensively studied, the mixing and conversion between excitons is only roughly known. Here, we observed changes in exciton formation in PTCDA as a function of layer number using time-resolved spectroscopy. We fabricated several layers of PTCDA through physical vapor deposition and determined their exciton lifetimes using time-resolved fluorescence. The appearance of excimers from layer 4 and above, along with a significant decrease in the fluorescence lifetime of charge-transfer excitons (CTE), confirms the conversion of CTE to excimers under specific conditions. This study not only showed the formation of excimers but also quantitatively identified the conditions for their formation. This could facilitate a better understanding of the exciton properties of organic crystals, which may have implications for various optoelectronic device applications, including OLEDs.

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Poster Presentation : **PHYS.P-170**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of Efficient Charge Transfer Rectification Molecular Photodiodes by Controlling Dipole Moments in Peptoid Systems

Ena Yun, Hohjai Lee*

Chemistry, Gwangju Institute of Science and Technology, Korea

Maintaining charge separation without recombination after electron transfer is crucial for device efficiency in the field of organic solar cells and optoelectronics. Conventional strategies to prevent charge recombination are increasing the distance or adjusting the angle between electron donor(D)-acceptor(A), but these methods also lead to a decreased charge separation.To overcome these limitations, we are trying to develop a new system based on the electric fields caused by dipole moments in peptide and peptide mimic structures, known as peptoid. The strength and direction of dipole moment in peptoid can be controlled by attaching the various residues to the peptoid. The dipole moment causes the electric fields that increase the rate of charge separation between the D/A, while decreasing the rate of the recombination. To develop the efficient charge transfer systems, the efficiency of electron transfer between D/A, molecular orbitals for the peptoid system with various residues are evaluated by density functional theory (DFT)/time-dependent density functional theory (TD-DFT) calculations.The aim of this study is to develop a photodiode molecular system that shows charge transfer rectification, where electrons only flow from D to A without back electron transfer from A to D. These results can provide valuable insight for the development of high-efficiency devices in solar cells and optoelectronic devices.

Poster Presentation : **PHYS.P-171**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Microplastics Analysis with Macro-scale Hyper Raman Imaging System

Hyung Min Kim[*]**, Hyeonjeong Yoon**

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The extensive use of plastic materials, driven by their numerous advantageous properties, has resulted in a substantial surge in plastic consumption, and as a result, there has been a significant increase in the generation of primary and secondary microplastics. Microplastics are typically plastic particles or fragments that are less than 5 mm size. As concerns regarding the adverse impacts of microplastics on ecosystems and human health continue to escalate, there is a growing interest in microplastic analysis. In response to this, our study has developed a macro-scale hyperspectral Raman method aimed at swiftly quantifying and characterizing substantial volumes of plastics.By implementing this approach, we achieved remarkable success, obtaining Raman spectra for five different types of microplastics scattered over a 1.5 cm2 area in a mere 1000 seconds. Utilizing a machine learning method, we demonstrated the effectiveness in acquiring Raman spectra, even when microplastics are suspended in aquatic environment or adhered to metal mesh nets. These findings underscore the significant potential of our developed method for practical real-world applications. We are currently conducting experiments aimed at classifying microplastics, even when they are trapped on cellulose filters, utilizing this system. Our objective is to achieve classification of microplastics present in authentic natural samples.

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Poster Presentation : **PHYS.P-172**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Effect of Tacticity on Physical Properties of Polystyrene from Molecular Dynamics Simulation

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The rheological and mechanical properties of polymer systems are crucial not only for the practical performance of the material but also for the manufacturing process. In particular, the variation of tacticity plays a significant role in determining the properties of polymers, such as glass transition temperature, crystallinity, thermal stability, and mechanical strength.Polystyrene, one of the most industrialized polymers, is a polymer with tacticity dictated by the benzene ring. In this study, we investigated the physical properties of syn-, iso, ata-polystyrene using molecular dynamics simulations.The atomistic (united-atom) force field was employed as the simulation parameter for polystyrene, and the Green-Kubo relation with an equilibrium molecular dynamics method, was applied for the viscosity calculation.

Poster Presentation : **PHYS.P-173**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Epi and Forward-Scattering Stimulated Raman Spectroscopy of 2D Inorganic and Organic Crystals

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Stimulated Raman spectroscopy (SRS), a coherent Raman scattering technique, offers significant benefits such as label-free imaging and signal amplification. These benefits not only overcome labeling-induced artifacts but also address the challenge of the inherently small Raman scattering cross-sections. Leveraging these advantages, SRS emerges as a potent tool for the characterization of two-dimensional (2D) materials with low Raman cross sections. In this work, we explored the limits of sensitivity in both epi and forward-scattering geometries using 2D hexagonal boron nitride (hBN) as an SRS reference. To mitigate instrumental noise, we implemented in-line balanced detection for both geometries. We also present the first demonstration of SRS spectral acquisition and imaging of 2D molecular crystals, specifically using mechanically exfoliated 2D pentacene. This study paves the way for broadening the applicability of SRS across a diverse array of 2D materials.

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Poster Presentation : **PHYS.P-174**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Thickness-Dependent Excitonic Behaviors of 2D Tetracene Crystals at Various Temperature

Sangjin Han, Sunmin Ryu*

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

Recent studies on two-dimensional molecular crystals (2DMCs) revealed their unique physical, electrical, chemical, and optical properties distinct from their bulk counterparts. Molecular crystals are expected not only to manifest such size effects like the conventional inorganic 2D systems, but also enable diverse future applications. In this work, we exploited top-down mechanical exfoliation to form 2D tetracene (Tc) crystals and investigated their geometric and electronic structures using scanning probe microscopy and variable-temperature photoluminescence spectroscopy, respectively. Significant variations in absorption and emission spectra were induced as a function of temperature and thickness. The origins of the spectral changes will be explained in terms of phase transitions, trap states and electron-phonon couplings. We will also discuss the fate of molecular excitons confined in the 2D systems based on time-resolved photoluminescence measurements. The unique photophysical properties of two-dimensional Tc revealed in this work will lead to a deeper understanding of excitonic behaviors in low-dimensional molecular solids.

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Importance of solvent and relativistic effects on the accurate description of the excited state structure of complex containing Hg2+ ion

Dae-Hwan Ahn, **Jong-Won Song***

Chemistry Education, Daegu University, Korea

Quantum chemical calculation to obtain the high accuracy excited state structures of complexes containing heavy metal ions is challenging due to the relativistic effect as well as large number of electrons included in the metal ions. Recently, we tried to reproduce the fluorescence spectra of the tetraphenylethene–bis(thiophen-2-ylmethyl)amine (TPE-BTA) containing Hg2+, which shows aggregation induced emission (AIE) fluorescence for the detection of Hg2+ [1], in order to analyze its emissive mechanism occurring in the excited state. However, DFT calculations showed too small energy differences between the ground (S0) and the first excited (S1) states following increased distance between sulfur of thiophene and Hg2+ in gas-phase, which made it difficult to obtain optimized excited state structures of S1. Therefore, we performed time-dependent (TD) DFT calculations using LANL2DZ, as a representative effective core potential (ECP) method, and Sapporo-DKH3-TZP-2012, as an all electron (AE) basis set, using DKH3 relativistic calculations for the Hg2+ to obtain potential energy surface (PES) of the ground and excited states following distance between thiophene and Hg2+.In this study, we found that the solvent effect with water considered using polarizable continuum model (PCM) with LANL2DZ basis set produces an appropriate energy gap between the S0 and S1 states, which results in stable potential well between thiophene and Hg2+ in the S1 state and eventually made us obtain the fluorescence spectrum which coincides with the experimental observation. Our study strongly suggests that both the solvent as well as relativistic effects are significant in calculating structures optimized in the excited state, in particular, containing Hg2+.[1] Anal. Chim. Acta 1148 (2021), 238178.

Poster Presentation : **PHYS.P-176**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancing Solvent Deoxygenation Efficiency: A New Inert Gas Bubbling Approach with Ventilation Path Addition

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Oxygen is an essential molecule for sustaining vital activity in most living things. O_2 is abundant in the atmosphere, making up about 21%, but researchers in many fields often struggle to create O_2-free environments. This is because oxygen's high reactivity can lead to unexpected reactions or reduce the yield of a product. Deoxygenation in a solvent is a common process in research labs, and several different methods have been introduced for it: boiling, sonication, freeze-pump-thaw (FPT), and inert gas bubbling. The FPT is widely considered to have the best deoxygenation efficiency (DE), but it needs a cold reservoir such as liquid N_2 and a high-performance vacuum pump, and the process must be repeated several cycles for longer than 30 min. The inert gas bubbling, on the other hand, consists of a high-purity inert gas tank with a proper regulator connected to a needle for solvent bubbling, and is a popular method to remove O_2 because it is simple and safe, despite being less efficient than the FPT. In this poster, we demonstrate that an improved inert gas bubbling with ventilation paths in addition to the basic bubbling setup improves DE. In improved method, the high ventilation flow rate from ventilation path enhances the DE by increasing gas flow rate that minimizes the ambient O_2 contamination per unit volume of Ar. The DE was monitored in real-time during the bubbling process through changes in photoluminescence (PL) caused by O_2-sensitive phosphor, platinum(II) octaethylporphyrin (PtOEP). It was demonstrated that improved method highly reproducible yields O_2-removal efficiency as high as FPT method. Using a simple kinetic model based on the mass transfer, O_2-profiles during the bubbling were simulated and fitted to find that amount of oxygen in the Ar-bubble decreases with the increased vent rate.

Poster Presentation : **PHYS.P-177**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Exact analytical distributions for the number of biomolecules in the living cells.

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Dynamic fluctuation in the number of biomolecules is a fundamental aspect of the living organisms, characterized by their probability distribution function. We present a generalized master equation that captures the temporal behavior of the distribution under renewal birth death process. Shedding light on the dynamic behavior of biomolecule populations, it is expected to advance the understanding in fundamental phenomena in various fields, including synthetic biology, pharmacology, and personalized medicine.

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Poster Presentation : **PHYS.P-178**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

In-plane Mixed-Dimensional Heterostructures composed of Monolayer MoS_2 and Low-Dimensional Mo/Te Compounds

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Mixed-dimensional heterostructures formed by combining 2D materials and other dimensional (0D, 1D, and 3D) materials have received rapidly increasing attention due to the synergetic effects and additional degrees of freedom to heterojunction for high-performance optoelectronic devices. Here, we report a sequential chemical vapor deposition growth method for synthesizing in-plane mixed-dimensional heterostructures from 2D molybdenum disulfide (MoS_2) and low-dimensional molybdenum/tellurium (Mo/Te) compounds. The dimension, composition, and phase of Mo/Te compounds interfaced with monolayer MoS_2 are controlled by adjusting the Te atomic flux and growth time. In-plane 2D/1D MoS_2/Mo_6Te_6 and 2D/2D/1D MoS_2/2H $MoTe_2/Mo_6Te_6$ heterostructures were selectively obtained at a low Te flux, whereas in-plane 2D/2D MoS_2/mixed 2H-1T’ $MoTe_2$ and 2D/2D MoS_2/2H $MoTe_2$ heterostructures were selectively synthesized at a high Te flux. The dimension-, composition-, and phase-controlled synthesis method developed in this study will allow large-scale controlled fabrication of edge-contacted in-plane mixed-dimensional heterostructures.

Poster Presentation : **PHYS.P-179**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Revealing the electric double layer structure with constant bulk electrolyte concentration simulation

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Understanding the electric double layer (EDL) is important for the advancement of electrochemical systems for efficient energy conversion. However, the molecular-level explanation remains elusive, for example, understanding of the 'camel-to-bell shape transition' of a differential capacitance curve, which occurs when the bulk electrolyte concentration is increased. To investigate the influence of bulk electrolyte concentration on the EDL structure, we developed a simulation method called 'Chemostat', which maintains a constant bulk electrolyte concentration. Using this method, we simulated interfaces between 0.1 M NaF electrolyte and Ag(111) electrodes at various electrode potentials to analyze the EDL structures. Our simulations revealed differences in the total number of ions at the interface corresponding to different electrode potentials, emphasizing the importance of maintaining consistent bulk electrolyte concentration for accurately describing the EDL structure. We discovered that the double-hump characteristic observed at low concentrations merges into a single-hump shape at 0.1 M, accompanied by the movement of the anodic hump towards the cathodic hump. This phenomenon arises from the specific adsorption of anions at the inner Helmholtz plane (IHP), which excessively screens electrode charging at the interface. We believe that our novel method offers insights into various EDL structures under finite electrolyte concentration conditions, with potential applications in electrocatalysts, supercapacitors, and beyond.

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Poster Presentation : **PHYS.P-180**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Single Molecule Localization Microscopy Based on Cyanine Dye Photoconversion

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Single molecule localization microscopy (SMLM) has revolutionized the study of cellular structures by enabling imaging beyond the diffraction limit of light. Alexa647, a fluorescent dye in the Cy5 family, has been widely used in SMLM through photoswitching mediated by thiol adduct formation. Recently, a photoconversion phenomenon has been reported, in which Cy5 reacts with singlet oxygen and converts into Cy3. We aimed to utilize this reaction to obtain super-resolution images based on single-molecule localization. Currently, the conversion efficiency is very low, making it unsuitable for obtaining sufficient localization points to reconstruct super-resolution images. To address this issue, we propose two methods. The first method involves increasing the density of fluorescent molecules using proximity labeling, allowing SMLM to be performed even with low conversion efficiency. The second method involves adding intermediates and additives to increase the conversion efficiency. These approaches make it possible to reconstruct super-resolution images with sufficiently high localization density through photoconversion.

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Poster Presentation : **PHYS.P-181**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Characteristics of Electrical Resistivity and Conductivity in the Preparation of Antimony-Doped Tin Oxide Coating on TiO2 Microrods.

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TiO2 microrods were synthesized using ion exchange and controlled calcination methods. A systematic investigation was conducted to explore the applications of TiO2 microrods as electric painting materials. The TiO2 microrods have a length of 4-8 μm and a length-to-diameter ratio of 13-28. Compared with the other strategies previously used for the synthesis of TiO2 microrods, it was found that large-scale production was possible under mild reaction conditions, which represented a facile and mild route for industrial production and expanded the versatile applications of TiO2 microrods. Additionally, one-dimensional conductive TiO2 rods coated with antimony-doped tin oxide (ATO@TiO2) were prepared using a hydrothermal coprecipitation method. Specially, cetyltrimethylammonium bromide (CTAB) surfactant was used as an interfacial reactor to form sufficient active groups on the surface of TiO¬2 rods. 0.2 g ATO@TiO2 rods were compression molded under a pressure of 2 ton for 3 min to form a disk with a diameter of 1.3 cm. And the ATO@TiO2 rods exhibited a resistivity of (70 ± 0.5 Ω cm). The morphology and composition of ATO coated TiO2 microrods were characterized using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX), while the resistivity of ATO@TiO2 was measured by a resistivity meter (4-point probe).

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Poster Presentation : **PHYS.P-182**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Polarized Absorption Spectroscopy of 2D PTCDA Crystals Grown on Graphene and Hexagonal BN

Kyungtaek Oh, Sunmin Ryu*

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The fate of excitons in a semiconductor is governed by its band gap and their binding energy, which are influenced by the dielectric screening. Excitons in two-dimensional (2D) systems are more strongly bound for reduced screening and can be tuned by engineering the effective dielectric constant [1,2]. In this work, we investigate how the reduced dielectric screening affects molecular excitons residing in 2D molecular monolayer and explore the possibility of their Coulomb tailoring. Using physical vapor assembly, we prepared 2D crystals of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) on top of several-layer hexagonal BN and graphene [3]. The excitonic absorptions obtained by angle-resolved differential reflectance spectroscopy revealed Davydov splitting in Frenkel-type S0-S1 vibronic transitions for 1L PTCDA without charge transfer mixing. The presence of graphene induced substantial spectral changes in Frenkel excitons: red-shift, broadening and reduced Davydov splitting. We will discuss their mechanistic origins and future investigation using variable-temperature and polarization-resolved methods. [1] : Raja, A., Chaves, A., Yu, J. et al. Coulomb engineering of the bandgap and excitons in two-dimensional materials. Nat. Commun. 2017, 8, 15251[2] : Tebbe, D., Schütte, M., Watanabe, K. et al. Tailoring the dielectric screening in WS2–graphene heterostructures. npj 2D Mater. Appl. 2023, 7, 29[3] : Kim, D., Lee, S., Park, J. et al. In-plane and out-of-plane excitonic coupling in 2D molecular crystals. Nat. Commun. 2023, 14, 2736

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Poster Presentation : **PHYS.P-183**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Advanced Detection and Characterization of Microplastics in Aqueous Environments Using Bright Field-Line Illumination Raman Microscopy

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Growing concerns regarding the environmental and human health impacts of microplastics necessitate improved detection and characterization methods. A significant amount of microplastic waste enters the environment and eventually makes its way into the oceans. While advancements in wastewater treatment technology mitigate some microplastic pollution, a significant portion persists in aquatic environments, as particles degrade below 1 micron and enter the nanoscale. Raman spectroscopy offers a valuable tool for microplastic analysis due to its low water interference, but its limited sensitivity presents challenges in observing the morphology of particles smaller than 5 microns. To address this, a comprehensive understanding of microplastics in aquatic environments and complementary techniques are necessary. We propose the application of bright field-line illumination Raman microscopy, enabling simultaneous analysis of both chemical composition and morphology. Our study successfully employed this method to observe and distinguish between three types of microplastics (polypropylene, polyethylene, and poly(methyl methacrylate)) ranging from 0.7 to 10 microns in water. Further, machine learning integration facilitated accurate material differentiation. This approach demonstrates significant potential for practical application in environmental monitoring and microplastic detection within aquatic ecosystems.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Circular Dichroism Spectroscopy of (3R,4S)-3-Hydroxy-4-phenyl-2-azetidinone

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We obtained the electronic circular dichroism (CD) spectra of (3R,4S)-3-Hydroxy-4-phenyl-2-azetidinone (HPA) of the origin band of the S_0-S_1 transition using dual-beam resonant two-photon ionization circular dichroism (R2PICD) spectroscopy. The dual-beam R2PICD spectra of HPA exhibited well-resolved electronic CD bands. These CD values can help to decide the chirality of each chiral center. Quantum calculation results confirmed that three conformers are possible. Comparing the IR-ion dip spectrum result with the calculated one, it was confirmed that it exists as a single conformer. The rotatory strength values of each origin band were estimated using time-dependent density functional theory (TDDFT) calculations and compared with the CD values of the origin bands.

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Poster Presentation : **PHYS.P-185**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Graph-Based deep learning strategy for prediction on properties of multicomponent system

Seongmin Yoo, Ji-Hyun Kim[1,*], Jaeyoung Sung[1,*]

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[1]*Department of Chemistry, Chung-Ang University, Korea*

It is a complex task to predict precise physical properties of multicomponent system with significant scientific and industrial relevance. Conventional computational or theoretical methods requires extensive computational resources and may not capture the complex interaction in chemical mixtures. Furthermore, machine learning strategies often fail to accurately account for the intricate interactions and compositional variability inherent in chemical mixtures. This limitation is particularly prominent in industrial applications as well as science, where quick and accurate property predictions are essential for process optimization and quality control. This study aims to develop a deep learning-based approach to predict the physical properties of binary chemical mixtures. We constructed a deep learning model that utilizes graph neural networks, training the model on both experimental and computational data. The model focuses on incorporating the fraction of each component in the mixture and the environments of components as key features for prediction, aiming to provide a more accurate and computationally efficient solution. Furthermore, addressing the challenge posed by the limited availability of desired property data, we leveraged transfer learning to utilize chemical embedding from graph convolution trained on relatively extensive datasets. The deep learning strategy developed in this study offers a promising avenue for the accurate, efficient prediction of physical properties in binary mixtures.

Poster Presentation : **PHYS.P-186**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Protein-Ligand interaction of the OR2AT4 as a target of acute myeloid leukemia

Seon Bin Song

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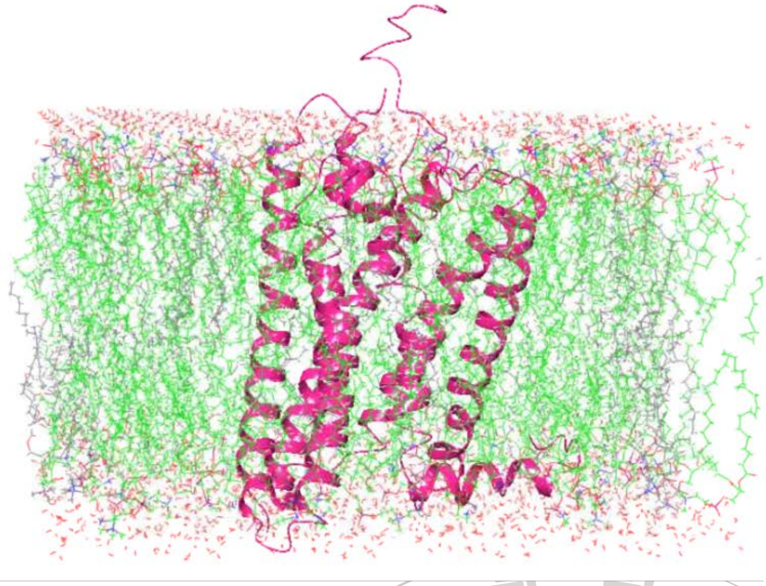
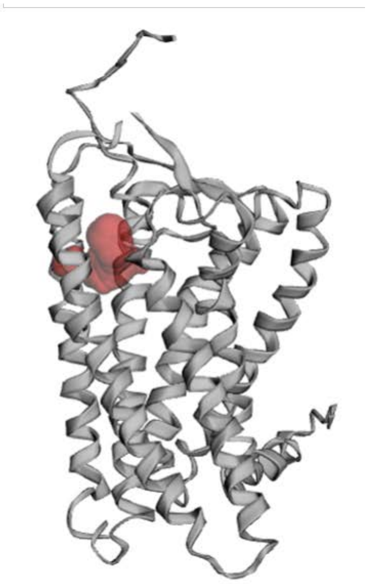
Through the first crystal structure of the olfactory receptor was revealed, the researcher interesting in the olfactory receptor has the opportunity to accelerate the investigation of the structural function and the application. OR2AT4 is one of the olfactory receptors but is especially expressed in the white blood cells and the skin cells. Although the relevant treatment function of OR2AT4 for acute myeloid leukemia, the unrevealed crystal structure of OR2AT4 makes it hard to investigate and improve the affinity even with an effective ligand, sandalore. In this work, we conduct the homology modeling of OR2AT4 and molecular dynamics simulation to define the binding site and the ligand interaction characters. We prepare the 3D structure of OR2AT4 from I-TASSER that gives the reliable 3D structure for the membrane protein like G-Protein Coupled Protein which OR2AT4 belongs to. With the molecular dynamics simulation, we expanse the expected binding site and perform the docking to identify the ligand interaction residue. The determination of the protein-ligand interaction character of OR2AT4 gives insight into the enhancing the treatment function of OR2AT4 and offers a possibility to facilitate the examining the distinctive function of other olfactory receptors.





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Poster Presentation : **PHYS.P-187**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Advanced Activity and Selectivity of CO2 Conversion on Bi2S3-Derived Bi Nanoplates

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Various electrocatalysts have been extensively studied for their ability to selectively produce desired products by electrochemical CO2 reduction reaction (CO2RR). The electrocatalytic CO2RR is difficult to lower the activation energy due to the high thermodynamic stability of CO2, and it is usually accompanied with competitive reaction in aqueous media; hydrogen evolution reaction (HER). Most bismuth-based catalysts have shown relatively high selectivity for formate production, but it still suffers from low catalytic activity. In this study, we found that Bi nanoplates derived from Bi2S3 exhibit superior electrocatalytic activity and selectivity towards formate (HCOO-) generation compared to metallic Bi in electrochemical CO2RR. To investigate the enhanced electrocatalytic properties of Bi2S3 derived Bi, we used DFT to analyze various kinds of defective surface of Bi and reaction mechanism on these surfaces.

Poster Presentation : **PHYS.P-188**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

To improve photocatalytic performance, metals are doped into g-C_3N_4 and fabricate electrodes that apply them to photoelectrochemical reactions

Kyung suh Kim, **Myung Jong Kang***

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Photocatalysis is an eco-friendly energy source that utilizes solar energy and has attracted great research interest because it can solve environmental problems. Graphitic carbon nitride (g-C_3N_4), one of the photocatalysts, is synthesized through a facile high-temperature reaction of melamine, urea, and dicyandiamide (DCDA). g-C_3N_4 composed of earth-abundant element, it is not only economical and environmentally friendly, but also has high chemical and thermal stability and a band gap suitable for absorbing visible light from solar energy. However, it has disadvantages such as high electron-hole recombination and low surface area. Metal doped g-C_3N_4 can overcome these disadvantages and improve photoelectrochemical efficiency. In this study, we analyzed their structures and photocatalytic properties and studied the fabrication of photoelectrodes that can be applied to photoelectrochemical reactions.

Poster Presentation : **PHYS.P-189**
Physical Chemistry
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Polarization-Dependent Plasmon Coupling in Gold Nanorod-Gold Nanosphere Core-Satellite Nanoassemblies

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Gold nanoparticles have unique properties such as bright visible color, creation of localized electric fields, generation of hot charge carriers, and emission of heat. These properties offer a wide range of applications from bioimaging, colorimetric sensing, to surface-enhanced spectroscopy. Plasmons, collective oscillation of free electrons, are at the heart of all of these phenomena. Resonant excitation of plasmons is a prerequisite to induce these properties. Assembling nanoparticles is a great way to tune the plasmon resonance. Plasmon coupling occurs through the interaction between nanoparticles in close proximity. Recently, we explored plasmon coupling in gold nanorods (AuNRs), as an anisotropic nanostructure, possess longitudinal (LO) and transverse (TR) plasmon modes. We have demonstrated that as gold nanospheres (AuNSs) attach to the end or side of AuNRs, plasmon coupling occurs selectively to LO or TR mode of AuNRs, respectively. In this study, we explore the possibility for preferential plasmon coupling for LO or TR mode for AuNR@AuNS core@satellite nanoassemblies using polarized light. We observe that the LO mode coupling mostly occurs when the light is polarized along the long axis of the AuNR. The LO mode coupling is not excited at all when the light polarization is perpendicular to the long axis. Surprisingly, the TR mode coupling, although much weaker compared to the LO mode coupling, occurs most strongly when the light is polarized along the long axis. This is presumably because the optically bright LO mode of the large AuNR is so dominant in the plasmon coupling that the interaction between the dipolar LO mode and induced dipoles of AuNSs is stronger than the interaction between the TR mode of a AuNR and the bonding dipoles of AuNSs.

Poster Presentation : **PHYS.P-190**
Physical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Method for Fabricating MgAl-layered Double Hydroxide Electrode for Photoelectrochemical Reaction Using Spin Coating

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Layered Double Hydroxide (LDH) is an anionic clay, structured as a double hydroxide composed of layers, typically consisting of metal layers with positively charged ions. Furthermore, it usually comprises metal layers with ions carrying positive charges, arranged in between an intermediate layer of anions that trap these metal ions. This structure bears a resemblance to that of brucite. The LDH structure features an ionic solid consisting of a series of stacked layers, and the inserted anions are weakly bound, allowing for anion exchange between layers. Metal hydroxides and anions are arranged alternately, and various combinations are possible through metal trivalent cations and divalent cations, and the LDH nanostructure is freely formed due to excess anions. The properties of LDH vary depending on the number of octahedral metal ions and interlayer anions. The polymorphic features in the chemical formula (structural repetition and number of layers in the crystal system) allow for a wide range of physicochemical properties. The characteristic structure of LDH allows for various changes through changes in anion exchange, metal, anion, and manufacturing technology. It is considered an attractive material for various applications.In this study, the manufacturing method of MgAl-LDH material used as a photoelectrode was studied. When producing an LDH-structured photoelectrode, Mg ions and Al ions were used as divalent and trivalent ions of LDH. To obtain optimal conditions for manufacturing MgAl-LDH electrodes, LDH was synthesized using MgAl-LDH by coprecipitation, and the spin coating was performed by dropping the solution on the FTO substrate. During spin coating, parameters such as the spin coating RPM and the number and concentration of electrode layers were adjusted. The photocatalytic and electrochemical properties of the prepared MgAl-LDH electrode were evaluated by LSV. The surface

morphology and chemical composition of the MgAl-LDH electrode were analyzed through SEM and EDS. Finally, the structural properties of MgAl-LDH were determined through XRD analysis.

Poster Presentation : **PHYS.P-191**
Physical Chemistry
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Computational Study on Novel Penta Monolayer MPS (M = Ni, Pd, Pt) as Promising Optoelectronics and Thermoelectric Materials with Visible Light Absorption and High Figure of Merit

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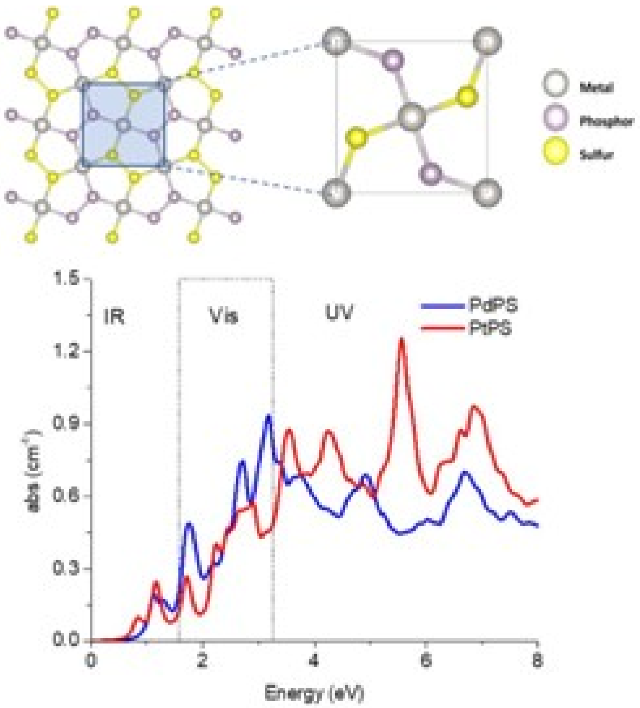
Penta monolayer MPS theoretically exists with its various structures. Phonon dispersion, mechanical properties, and molecular dynamics calculation prove structure stability of penta monolayer MPS using DFT Calculation. To determine the structure properly, we reported cis and trans configuration with square planar and distorted tetrahedral metal geometry for all penta monolayer MPS compounds. Our result presents penta monolayer MPS that exist in cis configuration are NiPS with distorted tetrahedral metal geometry and PdPS with square planar metal geometry. On the other hand, we found that penta monolayer MPS in trans configuration have square planar metal geometry only and are owned by PdPS and PtPS. All cis structures have no bandgap depending on HSE calculation. However, square planar metal geometry of trans configuration have narrow bandgaps. For trans-planar PdPS, optical properties are predicted to absorb visible light better than UV. BoltzTraP software package calculation exhibits high values n-type figure of merit for PdPS and PtPS (0.865 and 0.845). By owning high absorbing visible light, and high thermoelectric performance at room temperature, we deserve penta monolayer MPS will be potential optoelectronics and thermoelectric materials.


Metal
Phosphor
Sulfur
1.5
1.2
0.9
0.6
0.3
0.0
abs (cm⁻¹)
IR
Vis
UV
PdPS
PtPS
0
2
4
6
8
Energy (eV)

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Poster Presentation : **PHYS.P-192**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Hydrothermal Synthesis of Controllable WO3 Nanostructured Films for Enhanced Photoelectrochemical Efficiency on FTO Substrates

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Since Fujishima, A., & Honda, K. studied the photoelectrochemical decomposition of water using TiO2 under ultraviolet light in 1972, interest in harnessing clean energy using solar semiconductors has increased. Metal oxide photoanodes, including ZnO, TiO2, and WO3, are commonly used to harness clean energy through solar semiconductors. Among them, WO3 has emerged as a promising n-type semiconductor due to its excellent photon absorption ability and unique electronic properties. However, WO3 has disadvantages such as slow charge transfer at the electrode-electrolyte interface and fast electron-hole recombination. Regarding doping, nanostructure design, and heterojunction construction as solving the problems. Specially crafted nanostructures, with a variety of morphologies, exhibit superior properties compared to bulk materials, thanks to their distinctive structural characteristics. This technology emerges as a promising solution to surmount the aforementioned limitations. Nanostructured WO3 has been synthesized in various morphologically such as nanoplates, nanowires, nanoflowers, and nanosheets. However, achieving controllable direct growth of WO3 nanostructured films without capping agents and maintaining good adhesion to FTO substrates through hydrothermal synthesis methods remains a challenge. In this study, we successfully synthesized WO3 nanostructured films on FTO substrates using the hydrothermal synthesis method without a seed layer. Moreover, we observed the evolution of WO3 nanostructures with different reaction times at the same temperature, and the corresponding changes in photoelectrochemical (PEC) efficiency were monitored via linear sweep voltammetry (LSV).

Poster Presentation : **PHYS.P-193**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Unraveling Quantum Interference and Singlet Fission Dynamics in Conjugated Dimers with Heteroatom-Modified Benzene Linkers

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Singlet fission, a process in which one singlet exciton is converted to triplet excitons, represents a significant pathway for enhancing solar cell efficiency. Electron coupling is important to modulate singlet fission kinetics, and highly sensitive to orientation and linkage. Recently, our group reported that electronic coupling changes can be understood based on the quantum interference (QI). Pentacene is an archetypical singlet fission chromophore. Two Pc chromophores connected via benzene linker has been investigated thoroughly. However, the impact of heteroatom introduction into linker has remained less understood. In our research, we devised a molecular model system comprising trimetylsilyl-Pc dimers linked in 6,6’ and 2,2’ connections, with a specific emphasis on investigating the modulation effects caused by N-substitution and N,N’-disubstitution on the center benzene linker. Employing various quantum chemical simulations such as restricted active space with spin-flip (RAS-SF), time-dependent functional theory, and constrained density functional theory, we quantified the dynamics between nonadiabatic coupling (NAC) and QI phenomena. Our findings reveal pronounced through-space coupling in 6,6’-connected dimers, and therefore, the clear correlation between NAC and molecular electronics are not observed. Notably, the 2,2’-connected dimers displayed a significant correlation, governed by the positional and numerical variations of the substituted N atoms. There variations influenced the destructive QI effects and corresponded closely with the observed trends in electric conductance and NAC value.

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Physical Chemistry

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Fabrication of Non-Precious Transition Metal Carbide Catalyst for HER

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HER (Hydrogen Evolution Reaction) is attracting great attention as a new, eco-friendly and renewable energy source. However, the high overpotential associated with electrochemical water splitting in HER leads to significant energy consumption and reduced efficiency. Various materials are being investigated to alleviate these problems and improve the catalytic activity of HER. Among the various materials used for HER, noble metals like Pt, Ir, Rh, and Ru have relatively low overpotentials and excellent catalytic properties, but are expensive and difficult to mass produce. Accordingly, non-precious metal catalysts are emerging as an efficient and practical alternative for large-scale production. Among these alternatives, transition metal carbides (TMCs) have shown excellent catalytic activity in HER due to their high electrical conductivity and d-band electronic density states in this materials(TMCs) closely resemble those of Pt species, leading to catalytic behavior akin to platinum.In this study, our aim is to the high overpotential associated with HER and improve catalytic activity by depositing WC-Ni and WC-Ni-Co catalysts on tungsten tips. The electrode fabrication process involved electrodepositing these materials onto tungsten tips, Surface and compositional analysis were performed using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS).

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Physical Chemistry
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Exploring chemical reaction dynamics and mechanisms in photochemical reactions

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Understanding the vibrational modes involved in chemical reactions is paramount for elucidating reaction mechanisms. Distinguishing between reactive and non-reactive vibrational modes is crucial, as it allows for the identification of reaction coordinates and provides insights into molecular structural changes and reaction mechanisms as they occur. This study introduces an innovative experimental approach that employs femtosecond laser pulse analysis of coherent vibrational wavepackets (CVWs) to differentiate between these vibrational modes in real-time, offering a significant advantage in probing reaction dynamics.Focusing on photochemical reactions, particularly those in the excited state exhibiting non-Condon behavior, this research demonstrates how the anisotropic behavior of CVWs can indicate instances where the non-Condon approximation is invalidated by the reaction. By leveraging a model system with a two-dimensional potential energy surface encompassing both reactive and non-reactive modes, we simulate the progression of CVWs within the reactive mode and hypothesize the detection of these dynamics through polarization-dependent transient absorption experiments. The analysis of calculated polarization anisotropic TA signals enabled the distinction between reactive and non-reactive vibrational modes, showcasing the potential of femtosecond laser spectroscopy in identifying crucial vibrational modes involved in chemical reactions.Our findings propose a novel spectroscopic technique capable of distinguishing reactive vibration modes, providing a promising experimental methodology for exploring the mechanisms behind chemical reactions and enhancing our understanding of photochemical dynamics.

Poster Presentation : **PHYS.P-196**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Narrowing Nanogaps between Plasmonic Nanoparticles Using Plasma Treatment

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Nanogaps between the nanoparticles that constitute a nanoassembly determine the plasmonic properties of the nanoassembly. For instance, the nanogap distance tunes the resonance frequency of the optical response of the nanoassembly through plasmon coupling. Surface-enhanced Raman scattering is enabled only by the presence of nanogaps. Generation of hot carriers is significantly promoted in nanogap areas. Therefore, control of nanogaps is the key to the advancement of plasmonics. In this study, we find that plasma treatment is an effective way to narrow the nanogaps and eventually sinter the nanoparticles, leading to the production of newly shaped nanoassemblies. We synthesize 57 nm spherical gold nanoparticles (AuNSs) and assemble them into homodimers using a molecular linker with a distance of 1.3 nm. As we apply plasma, we observe that the plasmon coupling peak gradually redshifts, weakens, and then turns around to a blueshift and strengthens. Comparison of electron microscopy images reveals that plasma treatment narrows the nanogaps and causes the nanoparticles to merge. We prepare various nanoassemblies including heterodimers and core@satellite nanostructures using AuNSs, silver nanospheres (AgNSs), gold nanorods (AuNRs), and gold nanocubes (AuNCs). Applying plasma treatment to these nanoassemblies produces a new class of merged nanoparticles that have different plasmonic properties than nanoassemblies with gaps.

Poster Presentation : **PHYS.P-197**

Physical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Reversible and Electrotunable Assembly/Disassembly of Plasmonic Nanoparticles

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Plasmonic nanoparticles(NPs) show dramatically different scattering properties by the assembly/disassembly of the NPs due to the notable change between the collective and individual plasmonic modes, and reversible and on-demand control of such assembly and disassembly states of plasmonic modes is of great importance for potential optoelectronic and display applications. Control of assembly/disassembly of plasmonic NPs have been demonstrated by changing the pH, light exposure, or temperature. However, such cues are not very practical for device applications because of the limited reversibility and necessity of extended time. We report reversible and electrotunable control of assembly/disassembly of metal NPs by electrochemical redox reactions of copper complexes. The copper complex moiety is tethered to the surface ligands of metal NPs. The reversible control of assembly/disassembly of metal NPs was attained by switching the oxidation states between Cu(I) and Cu(II). Cu(I) state prefers tetrahedrally-coordinated complexes which form inter-NP sandwich structures and induces the assembled NP state. Whereas, Cu(II) takes octahedral ligand geometry which results in individually and freely dispersed NP state. Our control does not need external chemical reagents, and the reversible change can be made quite rapidly. The electrochemical control was also demonstrated by using a low operating voltage less than a couple of volts. We believe our design can be useful in optoelectronic display applications such as smart windows because it provides reversible bistability between transmittance and reflectance.

Poster Presentation : **ANAL.P-198**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Cyclone collection and IMS detection of explosives adsorbed in dust

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Sejong University, Korea

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

2,4,6-Trinitrotoluene (TNT), 1,3,5-trinitro-1,3,5-triazine (RDX), and pentaerythritol tetranitrate (PETN) are widely used explosives. Ion mobility spectrometry (IMS) is used for a field detection of explosives. If explosives are present with dust in a certain space, some of them can be adsorbed in dust. In this study, model dust samples mixed the explosives were prepared, and field detection of explosives by collecting dusts in a container was described. The model dust samples were dispersed in a fume hood and were collected using a cyclone collector equipped with a filter. Two types of filters, such as lens cleansing paper (LCP) and PTFE fabric sheet (TF), were employed. Then, the filter with dust was analyzed using IMS. The detection limits for two types of collection filters were analyzed. The results were compared when sprayed under various conditions, such as dust type, collection filter type, and spray site.

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Poster Presentation : **ANAL.P-199**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

A method for quantification of formaldehyde in phenolic resin using 13C NMR spectroscopy

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Analysis & Evaluation Team 1, KOLON INDUSTRIES, Korea

Unreacted formaldehyde remains in the phenol resin after completion of manufacturing. Since formaldehyde is a carcinogenic and hazardous substance, the amount of exposure to the human body must be minimized, so when manufacturing phenolic resin, a scavenger is added in the final process to reduce its content. The mainly used scavenger is urea, which reacts with formaldehyde to form urea-formaldehyde resin. Generally, formaldehyde is derivatized using DNPH (2,4 Dinitrophenylhydrazine) and analyzed by HPLC. Using this method has the advantage of being able to detect formaldehyde with a general ultraviolet detector, and paraformaldehyde in the form of self-polymerization by reacting with water can also be derivatized and analyzed by including it in the formaldehyde content. However, in the presence of urea-formaldehyde polymer, formaldehyde is decomposed and reacts with DNPH, so the residual amount cannot be accurately analyzed after the formaldehyde reduction process, and a value higher than the actual amount is observed. To solve this problem, we developed a method to accurately measure the content of formaldehyde remaining after urea injection using 13C NMR spectroscopy.

Poster Presentation : **ANAL.P-200**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Thermodynamics behavior of high-voltage olivine $LiFe_{0.4}Mn_{0.6}PO_4$ cathode

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Olivine cathodes exhibit stable voltage profiles, good thermal and electrochemical stability, high capacity retention, and reversible redox reactions, making them a favorable choice for use in high-performance Li-ion batteries, especially in applications such as electric vehicles and grid storage systems. In this research, the thermodynamics behavior of multicomponent olivine $LiFe_{0.4}Mn_{0.6}PO_4$ (LFMP) was evaluated. At low temperatures, the mobility of lithium ions within the olivine cathode material decreased and thus limited the rate of charge and discharge. In addition, the kinetics of the electrochemical reactions at the interface between the olivine cathode material and the electrolyte became more sluggish at low temperatures, resulting in higher polarization, increased internal resistance, and reduced overall battery efficiency. By providing a $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) solid electrolyte, the composite LFMP_LATP coated with carbon and LATP (LFMP_LATP@C_LATP) mitigated the inferior Li-ion diffusion to remarkably improve the capacity delivery and cycling stability, enhancing the low-temperature performance of the olivine cathode-based Li-ion batteries.

Poster Presentation : **ANAL.P-201**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis of and surface functionalization of VPO_5 anode material for Li-ion batteries

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High-performance anode materials for Li-ion batteries (LIBs) are essential to meet the requirements of large-scale applications. Here, we investigate the VPO_5 material, which exhibits a rich vanadium valence variation and a special crystal structure with electrochemically active VO_6 octahedron chains connected to inactive PO_4 tetrahedra. The VPO_5 anode material was successfully synthesized by a low-cost solid-state reaction process and exhibited satisfactory capacity for a Li-ion battery anode. More importantly, the capacity and cycling stability of the VPO_5 anode were significantly improved by providing fast Li-ion and electron channels made of carbon and $Li_{1.3}\ Al_{0.3}\ Ti_{1.7}\ (PO_4)_3$ solid electrolyte. Such an arrangement enhanced the conductivity to significantly improve the capacity delivery. In addition, the presence of carbon and $Li_{1.3}\ Al_{0.3}\ Ti_{1.7}\ (PO_4)_3$ could provide an artificial solid electrolyte interface to stabilize the cycling performance of the VPO_5 anode material. The development of VPO_5 with the coating strategy demonstrated a potential high-performance material for practical use in LIBs.

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Poster Presentation : **ANAL.P-202**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Novel Prussian blue-graphene quantum dot (PB-GQD) nanoarchitecture as an efficient electrocatalyst for H2O2 reduction

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

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The electrochemical catalytic activity and stability in electrocatalysts are key factors for hydrogen peroxide (H2O2) reduction reaction. Herein, we propose a novel electrocatalyst consisted Prussian blue (PB)-graphene quantum dot (GQD) (PB-GQD) nanoarchitecture fabricated through an in-situ electrochemical method. The small and evenly grown PB nanoparticles (NPs) in the PB-GQD nanoarchitecture formed by electrostatic attraction and/or coordination interaction between iron cations of PB precursor and multivalent GQD polyanions showed enhanced electrochemical catalytic activity and stability for H2O2 reduction reaction. The improved electrocatalytic performance of the PB-GQD nanoarchitecture can be attributed to fast heterogeneous electron transport, abundant electrochemically active sites, and short mass transfer lengths. Notably, GQD's presence, rich with hydroxyl (–OH) and carboxylic (–COOH) groups, mitigates the decomposition of PB NPs into Fe(OH)3 in neutral or higher pH solutions. We believe that our study on the PB-GQD nanoarchitecture will serve as another signpost in the exploration of highly active electrocatalysts and electrode active materials for electrochemical systems.

Poster Presentation : **ANAL.P-203**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

SERS Sensor Based on CRISPR/Cas12a for coronavirus disease detection: Application to SARS-CoV-2 diagnosis

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In recent times, the world has faced a pandemic caused by various coronavirus diseases. For the effective diagnosis and control of the pandemic, it is imperative to develop a rapid, reliable, and easily applicable diagnostic method. In this study, we report a surface-enhanced Raman scattering (SERS) Sensor Based on Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/Cas12a, utilizing Au nanowires, and apply it to the diagnosis of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). Utilizing Hairpin Probe-Mediated Isothermal Amplification (HIAmp), the detection method generates a substantial quantity of double-stranded DNA products, which are selectively recognized by the Cas12a/crRNA complex in the presence of target RNA. Subsequently, the activated CRISPR/Cas12 cleaves Cy5-labeled single-stranded DNA attached to Au nanowires, consequently reducing SERS intensity. This innovative SERS Sensing Based on the CRISPR/Cas12a method is anticipated to make a substantial contribution to the precise diagnosis of SARS-CoV-2, expanding the application of the CRISPR/Cas detection system.

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Poster Presentation : **ANAL.P-204**

Analytical Chemistry

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CRISPR/Cas-assisted Nanowire SERS Sensor for Detection of African Swine Fever Virus

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African swine fever virus (ASFV) is a highly contagious and deadly disease that affects both domestic and wild swine, causing severe economic losses. Thus, the development of a rapid and sensitive detection method is crucial. The clustered regularly interspaced short palindromic repeats (CRISPR)-Cas12a system has gained considerable attention in molecular diagnostics due to its sensitivity, specificity, and broad applicability. In this study, we report CRISPR/Cas12a-assisted Au particle-on-wire systems as a SERS sensing platform for accurate and sensitive detection of ASFV. In the presence of target DNAs, Cas12a/crRNA complex activates the cleavage of the linker single-strand DNA, resulting in a decrease of SERS intensity. Conversely, in the absence of target DNAs, the Au particle-on-wire structure is formed and SERS hot spots are created at the gaps of NW and NPs, resulting in a increase of SERS intensity. This study offers a practical method for rapid infectious disease diagnosis and is anticipated to be applied as a sensor for detecting various diseases.

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Poster Presentation : **ANAL.P-205**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

A Strategy to Enhance the Photoconversion of Organic Molecules via Host-Guest Interactions

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Plasmonic metal nanoparticles exhibit unique optical properties through a strong interaction with light, known as localized surface plasmon resonance (LSPR). Additionally, nanoscale plasmonic particles have exceptional catalytic activities due to their high surface area and active sites. Consequently, plasmonic nanoparticles can function as photocatalytic materials under visible light. When exposed to visible light, gold nanoparticles (Au NPs) generate hot charge carriers that can trigger redox reactions of organic molecules. The rate of photocatalytic reactions is highly influenced by the rate of charge transfer between the donor and acceptor, which is proportionally dictated by their distance. In solution, however, the donor-acceptor distance is randomly distributed, limiting the kinetics of photocatalytic reactions. In this study, we introduced a host-guest interaction by capping β-cyclodextrin onto the surface of Au NPs to enhance the photoconversion efficiency and stability. Organic molecules are included into the hydrophobic cavity of β-cyclodextrin through the host-guest interaction, maintaining a close and consistent distance between Au NPs (donor) and organic molecules (acceptor). After the reaction, the resulting products were verified to have been converted into oxidized form and β-CD@Au NPs showed faster photoconversion rate than Au NPs functionalized with aliphatic ligands.

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Poster Presentation : **ANAL.P-206**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthesis of Bimetallic Nanoclusters for Photocatalytic Organic Reactions

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In recent years, atomically precise noble metal nanoclusters have emerged as a new and intriguing class of nanomaterials in nanoscience research. Nanoclusters, exhibiting quantum confinement effects with ultra-small size regimes and electron structures resembling molecular-like quantum effects, have attracted broad interest in diverse applications such as sensing, optical, and catalysis. Bimetallic nanoclusters, incorporating two metals in the form of alloys or compounds, can possess unique electronic and geometric structures, showcasing distinctive catalytic properties. In this work, we synthesized narrowly distributed bimetallic nanoclusters (Au/Pt) with varying atomic ratios through the simultaneous reduction of two metal precursors in the presence of both solvent and capping agents. The synthesized bimetallic nanoclusters were then utilized to investigate a photocatalytic organic reactions such as, urea derivative synthesis. The bimetallic nanocatalysts and reaction products were characterized through FE-TEM, GC-MS, and NMR.

Poster Presentation : **ANAL.P-207**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Determination of equine urinary androgen by liquid and 4-spot dried urine with hyphenated mass spectrometry

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Testosterone(T) is a primary androgen in males, and the level of T in horses is being controlled in horseracing because of its anabolic effect. Some horses that are not properly trained are hard to collect sufficient volume of urine from, creating unexpected obstacle for drug testing. We developed a method for determination of testosterone using 4-spot dried urine, and the result was compared with our formerly developed in-house method for liquid urine. 12 urine samples from male horses were tested. 20 μL of urine was spotted onto Whatman™ 903 filter paper, air-dried for 12 hours, and cut out. The spots were allowed to be extracted by extraction solvent and underwent enzymatic hydrolysis for deconjugation of glucuronides and sulfates. After additional SPE cleanup procedure, quantitative analysis was carried out by UHPLC-Q-Orbitrap MS. Chromatographic separation was achieved by employing C18 reversed-phase column and a conventional binary solvent gradient. The mobile phases were water with 0.1% (v/v) formic acid and methanol with 0.1% (v/v) formic acid. Liquid urine samples for GC-MS/MS analysis underwent SPE, methanolysis for deconjugation, LLE and derivatization(heptafluorobutyration). QC accuracy(% RE) and limit of quantitation(LOQ) of DUS test was 6.28% and 10 ng mL^{-1}, respectively and r^2 value of the calibration curve was 0.951. Intraclass correlation coefficient(ICC) between the methods was 0.783.

Poster Presentation : **ANAL.P-208**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Stability and sensitivity enhanced paper-based nonenzymetic label-free SERS biosensor for glucose detection

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[1]*Chemistry, Kongju National University, Korea*

Glucose detection has an essential diagnostic importance for diabetes control and monitoring. In this work, we have fabricated a stability and sensitivity enhanced paper based nonenzymatic and label free SERS biosensor for glucose detection. The SERS biosensing platform is fabricated by modifying the cellulose paper (CP) with a naturally derived polymer, chitosan (CS), followed by depositing enormous amount of plasmonic silver nanoparticles (AgMPs) on CP/CS and finally forming a self-assembling monolayer of mercaptophenylboronic acid (MPBA) on CP/CS/AgNPs. The SERS platform is characterized by SEM EDX, and XRD techniques. The glucose detection is achieved by monitoring the intensity of C-S stretching band and 1072 cm^{-1} in MPBA, which is gradually increased with increasing concentration of glucose due to the increased orientation change of MPBA on AgNPs. The results show that the proposed glucose SERS biosensor exhibits high sensitivity with a limit of detection (LOD) of 0.74 mM and linear dynamic range between 1.0 and 7.0 mM. The practical application of this SERS biosensor for the glucose detection in real samples are currently in progress.

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Poster Presentation : **ANAL.P-209**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of a nucleic acid extraction device based on photothermal magnetic nanoparticles

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Nucleic acid extraction, a pivotal process in molecular biology, finds diverse applications ranging from diagnostic assays to cutting-edge research endeavors. However, conventional extraction methods often encounter challenges such as complexity, time consumption, and limitations in on-site deployment. This study aims to develop a device utilizing plasmonic nanoparticles for streamlined and expeditious nucleic acid extraction. Plasmonic nanoparticles possess the capability to absorb light of specific wavelengths from an external light source, generating heat as a result. Leveraging this property, these nanoparticles can effectively disrupt cell membranes. The silica shell of plasmonic nanoparticles offers heightened stability and a vast surface area, facilitating efficient binding and extraction of nucleic acids. Furthermore, the magnetic properties of the nanoparticle core enable facile separation. This research endeavors to harness these characteristics in designing a straightforward device for nucleic acid extraction and validate its efficacy. Such a device holds promise for on-site nucleic acid extraction applications with substantial potential across various fields including medical diagnostics, environmental monitoring, and biopharmaceutical production.

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Poster Presentation : **ANAL.P-210**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Hyperspectral NIR measurement of dried seaweeds for determination of their protein contents

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Hyperspectral imaging has gained widespread attention across various sectors, including agriculture area, owing to its rapid detection speed and ability to measure large areas. However, a notable limitation arises when dealing with thin samples, as the interaction of NIR radiation with the sample may not be sufficient to produce component-specific spectra with good signal-to-noise ratios. To solve this problem, PTFE was employed as a sample measurement plate, since it is an effective beam-diffusing medium with high reflectance. Therefore, this approach induces a trans-reflectance sample interaction, thereby increasing the number of photons interacting with the sample. To evaluate the usage of this proposed scheme, the NIR measurement of dried seaweeds, thin samples, were performed to determine their protein contents. A total of 51 sheets of dried seaweeds was measured by using both hyperspectral NIR and conventional transmission NIR instrumentations. Among the hyper NIR spectra, the spectra obtained at the well-focused regions were separated by k-nearest neighbor algorithm for subsequent quantitative analysis. Also, the transmission NIR spectra were collected by scanning over a similar area in the sample with a moving stage. Finally, partial least squares (PLS) was executed using both acquired data and errors in the determination of protein contents were compared.

Poster Presentation : **ANAL.P-211**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Efficient feature extraction using convolutional autoencoder (CNNAE) for hetero spectral two-trace two-dimensional (2T2D) correlation maps and interpretation using Grad-CAM

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Two-trace two-dimensional (2T2D) correlation analysis, which uses a pair of spectra instead of a series of spectra, has been widely used for various studies in vibrational spectroscopic analysis. It has the advantage of maximizing even minute differences in the spectra. Meanwhile, a 2T2D map data has an excessive number of features, which limits its direct use for discrimination analysis. So, only data of a slice spectrum at v (n×1 features) is typically used for subsequent analysis. However, information from the remained slice spectra, which would be still valuable for a target analysis, will be lost in this case. Additionally, Grad-CAM was used to interpret feature extraction through CNNAE. Grad-CAM enables the identification of the specific features that the convolutional layer deems significant. With the proposed method, the NIR and Raman spectra of red pepper powers were employed for the discrimination of their geographical origins and following results were discussed.

Poster Presentation : **ANAL.P-212**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Polyethylene glycol for highly efficient enrichment of exosomes derived from human blood serum

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Exosomes are nanosized extracellular vesicles measuring between 30-120 nm, that originate in the endosomal pathway and play crucial roles in intercellular communication. Recently, the applications of exosomes in disease diagnostics, therapeutics, and drug delivery have gained significant interest. In this study, we present an approach for enriching and isolating serum exosomes using polyethylene glycol (PEG) precipitation technique. To remove cells and other large molecules from the serum, the serum was subjected to low-speed centrifugation at 2,000 × g for 30 min, followed by additional centrifugation at 12,000 × g for 45 min. The resulting solution was filtered to remove cells and cell debris. The filtered serum (500 µL) was mixed with PEG and incubated at 4°C for 30 min, followed by centrifugation at 1,500 × g for 30 min. The resulting pellet was then dissolved in 500 µL PBS solution. This procedure was repeated four times. The results from size exclusion chromatography of the samples without PEG enrichment revealed the presence of two peaks, which are probably both protein and exosomes. The later eluting peak disappeared during PEG enrichment, and the most abundant peak was assumed to be exosomes. These results were further confirmed by western blot and scanning electron microscopy. Utilizing the PEG precipitation technique proves to be highly efficient for enriching exosomes from blood serum, offering a cost-effective and efficient substitute for commercially available products.

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Poster Presentation : **ANAL.P-213**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Applications of AccuGC™100, portable GC-PID

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We introduce the portable gas chromatography AccuGC™100 developed by Bioneer Co., Ltd. Additionally, we present some experiments and their results aimed at exploring applications that can leverage its powerful feature of portability. AccuGC™100, with its special structure that mounts the sample concentrator tube as the sample injection port, boasts significantly enhanced detection limits, making it a portable compact device capable of diverse applications. We investigated the differences between diesel and gasoline using a combination of a general adsorbent Tenax and PID detector specifications. In addition to general adsorption tube for VOCs analysis in the air, we also developed an adsorption tube for analyzing ethylene concentration. We obtained experimental results showing that the signal intensity linearly varies with the concentration of ethylene gas. This adsorption tube can be utilized for precise measurement of ethylene concentration in places such as fruit warehouses.

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Poster Presentation : **ANAL.P-214**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

SERS-based assay of uropathogen using magnetic beads immobilized with gold nanoparticles

Kihyun Kim, Jaebum Choo*

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The current gold standard method for the diagnosis of urinary tract infection (UTI) is urine culture. However, this method takes at least two days to obtain assay results and usually requires additional complicated steps, such as biochemical tests, polymerase chain reaction (PCR), or mass spectrometry to confirm whether the isolated strain is the pathogen of interest. To address these issues, we developed magnetic beads immobilized with gold nanoparticles (MB-AuNPs) as a surface-enhanced Raman scattering (SERS) substrate. The MB-AuNPs offer several advantages, including excellent magnetic properties that simplify the assay procedures and good SERS properties resulting from densely packed AuNPs. By using these MB-AuNPs, we performed a sensitive and rapid SERS-based assay to detect the most common bacterial species causing UTI, E. coli.

Poster Presentation : **ANAL.P-215**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Highly sensitive detection of SARS-CoV-2 RNA using CRISPR/Cas13a-mediated SERS-based dual-flow assay strip

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The gold standard method for diagnosing SARS-CoV-2 target gene is RT-PCR. However, amplifying the target gene requires a reverse-transcription and thermocycling process, taking approximately 3-4 hours. Due to the rapid spread of the virus, the lateral flow assay (LFA) strip is also employed as a diagnostic method. This approach is quick and simple but exhibits a high false-negative rate due to limitations of detection sensitivity. The trans-cleavage activity of the CRISPR/Cas system has recently demonstrated excellent potential for sensitive and rapid detection of the target gene. In this study, we developed a CRISPR/Cas13a-mediated SERS-based dual-flow assay strip sensor to detect SARS-CoV-2 RNA directly. Initially, CRISPR/Cas13a reaction occurred through the first channel, followed by the sequential flow of SERS nanotag solution through the second channel. This sequential flow arrangement allows for both the CRISPR/Cas reaction and the SERS assay within a single chip, enabling the sensitive detection of SARS-CoV-2 RNA. Furthermore, by utilizing CRISPR/Cas13a system, direct detection of SARS-CoV-2 RNA is possible without the need for a reverse-transcription process. Consequently, our SERS-based dual-flow paper chip holds significant potential for point-of-care testing (POCT) by enabling the direct detection of target RNA through two distinct reactions within a single chip.

Poster Presentation : **ANAL.P-216**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Simultaneous analysis of 29 banned Illegal dyes in Tattoo ink by Liquid chromatography-Electrospray ionization- tandem mass spectrometry(LC-ESI-MS/MS)

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In tattooing, coloring agents are injected through microscopic holes in the epidermal layer of the skin and remain in the skin for a long period of time, so it is very important that the dye for tattoo does not contain carcinogenic or allergenic dyes. However, there are no established analytical methods for the 35 tattoo dyes that are legally banned in South Korea. In addition, illegal dyes are divided into various classes according to their structural properties, acidic, basic, disperse, solvent, and pigment classes. Since each class has different physico-chemical properties, simultaneous analysis of all classes of illegal dyes is challenging. In this study, we developed an analysis method for the simultaneous qualitative and quantitative analysis of 29 dyes out of 35 illegal dyes, using liquid chromatography-electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS). The sample preparation procedure was optimized to increase the recovery rate in the simultaneous analysis of four classes of dyes. The analysis results by the developed method showed good analytical performances, including linearity, sensitivity, accuracy, and precision. These dyes also could be used in cosmetics, textiles, food, etc. due to their cost-effectiveness and intense colors. Therefore, this platform is expected to contribute to the improvement of current safety investigation and monitoring services by enabling simultaneous quantitative analysis of illegal dyes used in products for various purposes, not limited to tattoo inks.

Poster Presentation : **ANAL.P-217**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of Thermally Controllable Paper-Based Digital Microfluidics: Application to Electrochemical Detection of HPV

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Digital microfluidics (DMF) is a preferred lab-on-a-chip (LOC) platform in chemistry, biochemistry, and molecular diagnostics. To address integrating challenges with microheaters and sensors while ensuring simplicity and eco-friendliness, we propose a thermally controllable paper-based DMF (p-DMF) chip. Fabricated via inkjet printing with silver nanoparticles (AgNPs) and PEDOT:PSS conductive inks, it integrates electrowetting-on-dielectric (EWOD), microheaters, and temperature sensors for shuttle-run motion of droplets, heating, and temperature sensing, respectively. Despite variations in electrode designs and printing materials, all remain suitable for EWOD manipulation, ensuring smooth droplet motion. The p-DMF efficiently manipulated sample droplets, including merging, mixing, and transporting. The printed microheater generated heat to T > 100 °C (meander shape of 2 × 4 mm, R = 61.06 Ω), while the Seebeck coefficient of thermoelectric effect of the temperature sensor was 18.87 μV/K. As proof of concept, we developed a portable and automated device for strand displacement with enzyme-assisted signal amplification for electrochemical detection of HPV type16 cDNA. From sample introduction to detection, the experimental limit of detection was found to be at 0.001 pM.Keywords: Inkjet printing, Paper-based Digital microfluidics, microheater, thermocouple temperature sensor, Electrochemical detection

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Poster Presentation : **ANAL.P-218**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Novel mycophenolic acid precursor–based fluorescent probe for intracellular H_2O_2 detection in living cells and Daphnia magna and Zebrafish model systems.

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Reactive oxygen species (ROS) are oxygen–containing substances with high chemical reactivity, including well-known species such as superoxide anion, hydrogen peroxide (H_2O_2), hydroxyl radical, ozone, and singlet oxygen. H_2O_2, a byproduct of cellular functions, plays a crucial role in various physiological and pathological processes. Excessive H_2O_2 is associated with diseases such as cancer, aging, asthma, cardiovascular disorders, and a host of neurodegenerative conditions.The detection of H_2O_2 is essential for understanding its impact on health. Current methods include fluorescence probes, spectrophotometry, electrochemical assays, and colorimetry. Fluorescence probes, particularly those based on boric acid, offer a robust way to monitor H_2O_2 levels in living systems. In this report, we present a newly developed fluorescent probe utilizing a mycophenolic acid precursor. This probe enables the detection of H_2O_2 with a Limit of Detection (LOD) as low as 13 nM. The probe incorporates a boronate group within a mycophenolic acid precursor, which undergoes cleavage upon interacting with H_2O_2.The study introduces a novel fluorescent probe, LBM, combining aryl boronic acid and mycophenolic acid for selective H_2O_2 detection. Experimental results confirm LBM's effectiveness in detecting H_2O_2 with high selectivity, providing a promising tool for monitoring H_2O_2–related disorders.Live cell imaging and organism models such as Daphnia magna and Zebrafish, are invaluable research tools and in many cases crucial for validating the effectiveness of analytes such as H_2O_2 and the proposed detection method. The use of these models enhances the understanding and identification of disorders caused by excessive H_2O_2 concentration.

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Poster Presentation : **ANAL.P-219**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

The determination of inorganic mercury by solid phase extraction and inductively coupled plasma optical emission spectrometry

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The toxicity of mercury compounds is influenced by both their chemical structure and concentration. Accurate determination of these chemical species and their concentrations in diverse samples is crucial for assessing mercury toxicity. A novel approach for quantifying Hg(II) has been developed using an ion exchange membrane coupled with inductively coupled plasma optical emission spectrometry (ICP-OES). Hg(II) present in water is trapped by cation exchange membranes, and the Hg(II) loaded onto the membrane is leached and submitted for analysis by ICP-OES. The detection limit for Hg(II) was confirmed to be 0.5 mg/kg. The recovery efficiency for 1 mg/kg mercury standard solutions was excellent, reaching 96.3%. This method was successfully applied to analyze a certified reference material of Hg-spike water. These results indicate that SPE and ICP-OES provide sufficient analytical performance for the analysis of toxic inorganic mercury in water, with simple separation methods and low detection limits.

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Poster Presentation : **ANAL.P-220**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Implemented electroluminescent display on paper-based digital microfluidic device as an optical transducer for rapid spectral analysis

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Over the past few years, voltage-operated electrowetting-on-dielectric (EWOD) technology has garnered interest in various applications, including digital microfluidic devices. Specifically, paper-based EWOD devices, where conductive patterns can be fabricated through printing, offer numerous advantages, such as ease of fabrication and low cost. However, despite significant progress in the manipulation of droplets and mixing through surface-coated hydrophobic layers, sensing techniques for their analysis remain underdeveloped. Spectrophotometry, a classic method for chemical analysis of liquids, faces challenges in implementing light-emitting devices on paper substrates. In this study, we developed a paper-based device with a spectrophotometric light source that combines EWOD with alternating current electroluminescence (ACEL) transducers. The device harnesses the advantages of EWOD technology, allowing precise manipulation of liquid samples on a paper substrate, and ACEL transducers, which emit light when a voltage is applied. This ACEL transducer can emit light with an intensity of 9.8 mW/m2, enabling us to utilize spectral analysis within the visible light range, particularly focusing on the range of 430-550 nm. The synthesized iron chelate has been analyzed with it. As a result, we successfully demonstrated the same absorbance tendency as with UV-Vis spectrum, measuring each spectrum within a rapid 3 seconds. With further development and optimization, the integrated DMF p-chip is poised to revolutionize point-of-care testing, especially in fields requiring rapid and portable spectral analysis.

Poster Presentation : **ANAL.P-221**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Recent advances in preparing near-infrared molecular probes via indole incorporation.

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Fluorescent probes play essential roles in medical imaging, where researchers can select one of many molecules to monitor the status of living systems under investigation. However, only a few novel scaffolds that allow the in vivo detection of H2O2 are available now. Here, we report the first indole–incorporated NIR fluorescent probe Indo–H2O2 that allows H2O2 detection, which does so with a LOD of 25.2 nM. The pharmaceutical or medical sciences are interested in theranostics, and unique drug delivery systems (DDSs) that can track drug release in real time. Its ability to produce distinct signals upon drug release, providing information about the local drug dosage and its distribution in tissues, sets it apart from other DDS systems. Nevertheless, some of them might not work well with theranostic DDSs; the tissues that the DDS needs to enter may absorb light strongly in the 450–530 nm range. Therefore, the tissue penetration depth of light for this range is constrained. This problem might be resolved by the use of near-infrared chemical systems. Moreover, drug delivery systems often do not afford organ specificity; this makes drug delivery often unpredictable/nonspecific. Our probe (Indo–H2O2) features a boronate group on an indole scaffold that cleaves upon reaction with H2O2. A 5-membered malononitrile moiety was selected and incorporated on an indole scaffold to add to its near-infrared properties. The malononitrile moiety also reduces the reaction time (saturation within ~25 min) compared to other related probes. Herein, we provide a highly sensitive and selective fluorescent probe that detects H2O2 based on the ICT sensing mechanism. Indo–H2O2 was successfully employed in the endogenous and exogenous imaging of H2O2 in living cells. Indo–H2O2 also allows for real-time monitoring of H2O2 in vivo, particularly in the gallbladder (zebrafish). These findings offer the development of Indo–H2O2, a highly

sensitive fluorescent probe for the detection of H2O2, and a concept for incorporating indole scaffolds in novel fluorescent probe designs. Based on our previous probe Indo–H2O2, we came to know that, both of these issues might be resolved since the indole core of the compound shows its applicability in the near-infrared region and its availability in the gallbladder region of zebrafishReferences[1] Jain, N.; Sonawane, P. M.; Roychaudhury, A.; Park, S. J.; An, J.; Kim, C. H.; Nimse, S. B.; Churchill, D.G. Talanta, 269, 2024, 125459

Poster Presentation : **ANAL.P-222**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Study of Solvent and Temperature Parameters for Phthalates Screening using Thin Layer Chromatography (TLC)

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The use of four types of phthalates (DBP, DIBP, BBP, and DEHP) in electrical and electronic products such as semiconductors and displays has been restricted since 2019 in accordance with the 'Guidelines for Restriction of the Use of Environmentally Harmful Substances in Electrical and Electronic Products'(RoHS II). In order to detect phthalates in electrical and electronic products, GC-MS(Gas Chromatography-Mass Spectrometry), HPLC(High-Performance Liquid Chromatography), and Py/GC-MS(Pyrolysis/GC-MS) analysis methods were used. These methods are valuable for both qualitative and quantitative analyses, but they do require a significant amount of time. Quantification is difficult using the TLC(Thin Layer Chromatography) method, but qualitative analysis for screening purposes is possible in a short time and without an analysis device. However, since errors depending on the analysis method are large, standardization of the analysis method is necessary. In this study, the qualitative analysis results were optimized by using 7 types of phthalates (4 regulated, 3 expected to be regulated) and 4 types of solvents by polarity (EA, Acetone, MC, Hexane) in optimal ratios. In addition, the influence of the temperature factor was not considered in the existing TLC analysis, but in this study, the analysis method was optimized to ensure reproducibility while adding the influence of temperature.

Poster Presentation : **ANAL.P-223**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Photonic crystal synthesized by Self-Emulsion polymerization method for colorimetric thermo sensor

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Emulsion polymerization is an evolving method of polymer synthesis with various applications in paint, cosmetics, and construction materials. However, emulsion polymerization is a radical polymerization process using monomers, initiators, and surfactants. Therefore, impurities like surfactants can be difficult to remove, potentially negatively impacting the polymer's properties. To address this, in this study, we synthesized polymer photonic crystals via Self-Emulsion Polymerization (SEP) using only monomers and water-soluble initiators, without surfactants or stabilizers, offering a more environmentally friendly and straightforward approach. The bandgap of these photonic crystals can be altered based on particle size, allowing for the adjustment of structural colors. The SEP technique enables precise control over the size of the photonic crystal particles through various synthesis parameters such as the amount of monomer, initiator, and temperature, resulting in high color selectivity. In addition, the SEP synthesis technology enables the creation of photonic crystals that react at desired temperatures by mixing various types of monomers. Based on this, we developed a colorimetric thermo sensor with Remarkable optical stability and selectivity.

Poster Presentation : **ANAL.P-224**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of Multifunctional PCM Microcapsules with biocompatibility and Analysis of Physicochemical Characteristics

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Phase-change materials (PCMs) are substances that manage heat through phase transitions, offering significant latent heat for energy storage, making them valuable in construction, textiles, and energy transport. Despite encapsulation techniques mitigating toxicity, leakage, and chemical instability of PCMs, the safety of the encapsulating materials themselves continues to pose significant concerns. In this study, we developed PCM capsule materials with biocompatible and high thermal stability shells that can be used in various fields and analyzed their physicochemical properties. The emulsion polymerization method was used to encapsulate PCM, and Polymethylmethacrylate (PMMA), which has high thermal stability, biocompatibility, and chemical resistance, was selected as the wall material. The morphological structure was confirmed through microscopic images, and the size distribution and PDI were measured by DLS. These results showed the formation of capsule material with an overall uniform size of about 7.8 μm. Also, FT-IR measurements were performed, and the disappearance of C=C peak confirmed change in molecular structure due to polymerization, which indicated that the shell was formed well. To further analyze the structure of the synthesized capsules, we measured the 1D NMR and found that the peak signal of ester group and repeat unit structure of PMMA were identified, confirming that polymerization had occurred, and a specific structure and phase change of core could be assigned. In conclusion, the overall results demonstrated that the PCM capsule successfully formed a core-shell structure, indicating promising potential for diverse application. Future work will involve evaluating the thermal performance and stability of these capsules using TGA and DSC measurements.

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Poster Presentation : **ANAL.P-225**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Optimization of lecithin-encapsulated drug delivery system: Comprehensive NMR characterization and improved skin permeation profiles

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Polymeric micelles derived from self-assembled amphiphilic block copolymers represent a new paradigm in drug delivery system (DDS) due to their high delivery efficiency and biocompatibility, which enhance therapeutic efficacy and reduce side effects. This study synthesized a drug carrier (micelle/emulsion) using the amphiphilic polymer PEO-b-PCL and assessed their physiochemical changes via ^1H NMR, contingent on the type and concentration of lecithin additive. By measuring the T_2 relaxation time within these systems, we discerned that incorporating 10% symmetric lecithin into micelles and 10% into emulsions yielded optimal stability. Conversely, the greatest flexibility of micelles and emulsions with asymmetric lecithin was observed at 15% and 5%, respectively. Given these points, NMR-based T_2 relaxation time measurements provided deeper insight into how the structural properties of the additive affect the stability and flexibility of the drug transporter. Moreover, Franz cell assays were conducted on emulsions exhibiting optimal flexibility to confirm their skin penetration efficacy, thereby proving their viability for pharmaceutical applications. After applying the emulsions to the skin for 24 hours, their permeability was quantitatively analyzed by HPLC. In consequence, emulsions containing asymmetric lecithin exhibited significantly higher penetrability than those with symmetric lecithin. Accordingly, overall results demonstrate that core crystallinity, a key factor in the performance of drug delivery vesicles, can be effectively regulated by varying the type and concentration of additives and evaluated

with NMR. These findings contribute the way for designing advanced complex drug carriers, potentially offering strategic insights for improvement.

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Poster Presentation : **ANAL.P-226**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

One-step self-encapsulated perovskite quantum dot polymer film for high color purity down conversion film

Dong Gun Oh, Jin Woo Choi[*], Hongki Kim[*]

Kongju National University, Korea

Emission materials utilized in displays demand both high color purity and efficient photoluminescence characteristics. Consequently, perovskite quantum dots (QDs) have garnered significant attention due to their narrower emission spectrum and superior luminous efficiency compared to traditional organic materials. However, the mixing of perovskite QDs with different halide compositions leads to the diffusion of halide ions between them, resulting in an intermediate composition. Thus, a simple mixture of green MAPbBr3 QDs and red MAPbI3 QDs produces orange MAPbBrXI1-X QDs. In this study, we explore the fabrication of self-encapsulated QD-embedded optical films. During the thermal treatment of the polymer film, perovskite QDs precipitate within the polymer matrix and become encapsulated. To optimize the optical characteristics of the perovskite QDs film, we controlled the perovskite precursor ratio and concentration within the polymer. Finally, we successfully fabricated high color purity down-conversion photoluminescence sheets by depositing red perovskite QDs onto the films without the presence of halide ion diffusion issues.

Poster Presentation : **ANAL.P-227**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Quantitative Determination of Aromatic Amines Released from Azo Dyes in Tattoo Ink by Gas Chromatography-Electron Ionization-Mass spectrometry(GC-EI-MS) and tandem mass spectrometry(GC-EI-MS/MS)

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Dongguk University, Korea

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Azo dyes are compounds characterized by their vivid colors and provide excellent coloring properties. They are important and widely used as coloring agents in a variety of industries. The risk in the use of azo dyes arises mainly from the breakdown products that can be created in vivo by reductive cleavage of the azo group into aromatic amines. For this reason, several aromatic amines are classified as carcinogenic, and quantitative analysis of them in various household chemicals is essential. In this study, effective methods for determining hazardous aromatic amine products of azo dyes in tattoo ink products were developed by using gas chromatography-electron ionization-mass spectrometry (GC–EI-MS) and GC-EI-tandem MS (GC-EI-MS/MS). For the identification of the analytes one precursor ion and two daughter ions (multireaction monitoring, MRM) were selected and the GC-MS/MS parameters were optimized to achieve high sensitivity and selectivity. The developed method with GC-MS/MS showed superior analytical performances over conventional methods listed in international organization for standardization (ISO). Therefore, we expect that the method developed in this study can replace the current ISO methods and can be applied to a wide range of products containing dyes, not just tattoo inks.

Poster Presentation : **ANAL.P-228**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Chemical Fingerprinting Analysis of Pen Ink and Dyes by Matrix-assisted Laser Desorption Ionization and Capillary Electrophoresis

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Dongguk university, Korea

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There are many different substances present in commonly used pens. Even pens of the same color have very different types of dyes and polymers depending on the make and model, and the ingredients are not disclosed in detail due to patents. One of the key issues in forensic document analysis is determining which pen was used for two different documents or letters written with the same color pen and in the same handwriting. Therefore, to solve this problem, it is necessary to establish a database that can identify the type of pen based on the chemical fingerprint of the pen ink. In order to achieve this, we utilized matrix-assisted laser desorption ionization mass spectrometry (MALDI MS) and capillary electrophoresis (CE) as chemical fingerprinting analysis plaforms for pens. First, we optimized MALDI experimental conditions for MALDI MS including choices of matrix and extraction solvents mass spectra. Then, we collected MALDI mass spectra of pen dye standards and various pens to establish a database. For fingerprinting analysis for pens containing anionic dyes that are relatively difficult to analyze with MALDI MS, we performed additional chemical fingerprinting analysis with CE. We believe that the binary and highly orthogonal data obtained through MALDI MS and CE can contribute to improving the reliability of pen identification.

Poster Presentation : **ANAL.P-229**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

IL6-MagLISA: A Magnetoplasmonic Chemiluminescent Immunoassay for Quantifying Sepsis Biomarker

Huu-Quang Nguyen, My-Chi Nguyen, Haheun Yoo, Jaebeom Lee*

Department of Chemistry, Chungnam National University, Korea

Immunoassays such as ELISAs and lateral flow assays are widely acknowledged as the gold standard for detecting and quantifying biomarkers, offering unparalleled specificity and sensitivity. The integration of magneto-plasmonic nanoparticles (MagPlas NPs) into immunoassays holds promise for enhancing sample preparation, analyte enrichment, and biomarker detection for specific diseases. In this study, we developed a MagPlas-enzyme linked immunosorbent assay (MagLISA) for quantifying Interleukin-6 (IL6) to facilitate early sepsis detection, utilizing Fe3O4@Au core-shell MagPlas NPs as the substrate. Antibodies specific to human IL6 were conjugated to the Au nano-islands on the Fe3O4 substrate, enabling the design of flexible and robust immunoassays. Initial results from the chemiluminescent assay indicated that IL6 biomarker concentrations as low as 8.5 pg/well could be detected without sample preconcentration. In comparison to commercial ELISA methods, our developed assay offers numerous potential advantages in sample preparation, detection range, and storage conditions.

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Poster Presentation : **ANAL.P-230**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Investigation on Physicochemical Property and Structure of Human Hair Using ^{13}C Cross-Polarization Magic Angle Spinning NMR Spectroscopy

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Solid-state NMR is the most promising method for structural analysis of complex, solid biological tissues, and cross-polarization was used to increase the peak intensity of carbon. We aimed to investigate specifically the structural and mobility changes in human hair subjected to various cosmetic treatments such as bleaching, perming, dyeing, and straightening. In this study, ^{13}C CP-MAS NMR was performed to analyze the structure of α-keratin, a major component of hair, and $T_{1\rho}$ relaxation time was measured to evaluate the mobility of hair. ^{13}C CP-NMR spectra revealed variations in the metabolite as the number of hair bleaching steps increased. The area and linewidth of α-helix decreased and β-sheet increased in the carbonyl region, and the portion of cysteine decreased due to disulfide bond cleavage in the aliphatic carbon region, which is the side chain of amino acid. By observing clear $T_{1\rho}$ changes in α-helix and β-sheet of the hair, the shorter relaxation time of treated hair in α-helix suggests that the cosmetic procedure resulted in bond breaking and increased mobility. Further, the physicochemical properties of the hair were confirmed by various analytical instruments such as SEM, FT-IR and microscope. Ongoing work is focused on performing principal component analysis to qualitatively assess the condition of hair after chemical treatment. In conclusion, we would like to propose a new approach to develop an evaluation method using solid-state NMR and build a database based on it for the comparative analysis of different hair types caused by cosmetic procedures.

Poster Presentation : **ANAL.P-231**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Dynamic Nuclear Polarization of Onion-Shaped Silica Nanoparticles with Selective 29Si Isotope and Radical Enrichment

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Silica nanoparticles exhibit favorable attributes for developing 29Si MRI probes, featuring advantageous dispersion, biocompatibility, tunable size, and facile surface modification. However, challenges arise in detecting low-concentration species and low-γ nuclei using magnetic resonance spectroscopy. To address this, we explore the application of the Dynamic Nuclear Polarization (DNP) technique, known for amplifying NMR signals, however, the successful hyperpolarization with SiO2 NPs is hindered by the lack of intrinsic electronic defects. In this study, we introduce diverse onion-shaped SiO2 NPs (40 nm core@10 nm shell@10 nm shell) with selective 29Si isotope and TEMPO radical enrichment in distinct regions. The increased 29Si ratio enhances the magnetic resonance signal, and the embedding of free radicals facilitates particle polarization. Through detailed experiments, we establish the potential for self-polarization in DNP, advancing the development of SiO2-based 29Si MRI probes.

Poster Presentation : **ANAL.P-232**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of Light-Responsive Polylactic Acid for Sustainable Biodegradable Materials: Synthesis and Microcapsule Formation

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The escalating environmental impact of petrochemical-derived plastics and their subsequent accumulation in ecosystems have necessitated the exploration of biodegradable alternatives derived from renewable sources. Polylactic acid (PLA) has emerged as a promising candidate due to its renewable, biocompatible, and biodegradable nature. To advance the application of this polymer, our study aimed to develop PLA as a stimuli-responsive polymer (AZO-PLA) by incorporating a photo-switchable monomer (azobenzene, AZO) into the long-chain polymer. The light-switchable microcapsules were fabricated using a precipitation method afterward. The structures of PLA and AZO-PLA were characterized by 1H, 13C, and DOSY NMR spectroscopy. Results from 1H NMR and polymer end-group analysis confirmed the successful fabrication of low-molecular-weight (L)-PLA from lactic acid monomers. Furthermore, the attachment of light-responsive monomers to the PLA chain was validated by the appearance of aromatic signals in the NMR spectra of AZO-PLA. SEM and NMR techniques were employed to characterize the formation of microcapsules based on AZO-PLA, demonstrating the creation of small spherical capsules from the synthesized polymers. Future research will investigate the light-responsive properties influencing the structure of both polymers and capsules using UV-Vis and NMR analysis.

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Analytical Chemistry
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Development of Pumpless PCR and Paper-Based DNA Detection Sensor for On-Site Rapid Detection of Blue-Green Algae

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The green tide phenomenon, characterized by the rapid proliferation of cyanobacteria or blue-green algae in water bodies, poses a significant threat to water resources and human health through the production of harmful cyanotoxins. Monitoring techniques, such as polymerase chain reaction (PCR) and enzyme-linked immunosorbent assay (ELISA), have been developed to identify and quantify cyanobacteria species. However, rapid and accurate detection methods are also essential to provide a quick on-site examination without laboratory equipment. In this study, a pumpless PCR device has been developed to optimize the benefits of microfluidic PCR while simultaneously reducing the mechanical drawbacks associated with the need for an external pump. This portable pumpless PCR is an affordable technology capable of being used outside the laboratory for on-site analysis. In addition, a paper-based DNA sensor with fluorescence detection has been selected to provide a rapid detection system. The paper-based sensor leverages the specificity of DNA probes designed to target unique sequences within algae species of interest with a low amount of sample loads. This technology offers a cost-effective alternative to traditional detection methods and provides a practical and field-friendly solution for the early identification of harmful algae.Keywords: blue-green algae, cyanobacteria, pumpless PCR, paper-based sensor, DNA sensor, fluorescence sensor

Poster Presentation : **ANAL.P-234**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Probing Optical Characteristics and Chemical Interface Damping in Gold Nanorods via Cucurbit [6] uril Host-Guest Chemistry

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Gold nanoparticles (AuNPs) have attracted considerable attention in various fields due to their excellent compatibility with living organisms and stable chemical properties. They are particularly useful for facilitating processes like chemical interface damping (CID) when they interact with molecules adsorbed onto their surface. Despite their potential, research using host-guest supramolecular systems to control CID on AuNPs has been limited. This study introduces a new method for controlling CID on AuNPs using host-guest supramolecular complexes. We created a complex called CB[6]-BAPA, based on a well-known host molecule called Cucurbit [6] uril (CB[6]), which has the ability to encapsulate and release guest molecules. By employing this complex, we were able to modulate CID processes on AuNPs in a reversible manner. Through a series of experiments, we demonstrated how the CB[6]-BAPA complex could be used to control CID. By attaching amine groups from the complex onto gold nanorods (AuNRs) and then releasing CB[6] using an alkaline solution, we achieved precise control over the CID process. Changes in certain parameters during the experiments confirmed the successful formation of the CB[6]-BAPA complex and the release of CB[6]. Therefore, this study provides new insights and potential applications, such as in biosensing and drug delivery, by showing how reversible control of CID can be achieved using CB[6]-based host-guest complexes on individual AuNPs.Keywords: gold nanorods, localized surface plasmon resonance, chemical interface damping, cucurbit [6] uril, host-guest.

Poster Presentation : **ANAL.P-235**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Unraveling Plasmon Damping in Silver–Coated Gold Nanorods: Insight from Single–Particle Analysis and Damping Tuning

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A study about silver–coated gold nanorods (AuNR@Ag) remains a captivating area of research. In this study, the morphology and optical properties of AuNR@Ag is investigated. We examined the relation between surface damping and the thickness of silver shell on a single particle level. Utilizing Scanning Electron Microscope (SEM) and Dark Field (DF) Spectroscopy, we studied the near-infrared longitudinal peak in AuNR. We aim to finely adjust the bulk damping and radiation damping of AuNRs to understand the role of surface damping better. Notably, we observe visual changes in gold nanorods upon silver coating, accompanied by an increase in incubation time. SEM analysis reveals an increase in length and width following silver deposition. Energy-dispersive X-ray spectroscopy (EDS) confirms the deposition of silver with increasing content in a longer incubation time. DF Spectroscopy shows a distinctive blue shift and slight broadening. Adjustment in surface damping demonstrates a decrease with an increase in silver content. This study enhances our understanding of the interaction between silver and gold the interface

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Vibrational Circular Dichroism in Chiral Ligand Encapsulated Metal Chalcogenide Nanoparticles

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The utilization of nanoparticles composed of metal chalcogenides surrounded by ligands, which show a circular dichroism (CD) signal in the near-infrared (NIR) spectrum, is a promising avenue for optical studies. These nanoparticles are notable for their exceptional optical properties, tunable CD response through ligand modification, and their compatibility with biological tissues. This versatility makes them highly suitable for a wide range of uses, propelling advancements in fields like biological imaging, sensing, and the development of advanced optical devices. Ongoing research and development of the optical features of iron selenide (FeSe) quantum dots with chiral ligands are poised to push the boundaries of optical science, leading to groundbreaking discoveries in various scientific and medical fields.

Poster Presentation : **ANAL.P-237**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Study Competition between Plasmon Decay pathways of Gold Nanorods on Graphene

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We present an analysis of the electron transfer during interaction of gold nanorods with graphene layered on glass. Using single -particle dark field microscope we tried to observe surface plasmon resonance for gold nanorods and resulting broadening on full width half maximum of gold nanorods. This condition assigns that plasmon damping to charge transfer between plasmon generated hot electrons and the graphene that acts as efficient acceptor. Then we also tried to study the interaction of gold nanorod on graphene with pyridine. Where pyridine can cause plasmon damping on gold nanorods surface. Interestingly, we found that narrowing of the surface plasmon resonance for gold nanorods exposed graphene and pyridine. This result present competition of charge transfer for gold nanorods when interacting with graphene and pyridine.

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Analytical Chemistry

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Electrochemical Tuning of Hot-electron Generation and Chemical Interface Damping in Single Gold Nanorods

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Gold nanoparticles (AuNPs) exhibit the localized surface plasmon resonance (LSPR) property, which refers to the collective oscillation of conduction band free electrons when interacting with the electromagnetic spectrum. Gold nanorods (AuNRs), which have tunable size, shape, and structure-dependent plasmonic properties, experience LSPR energy loss when the organic molecules absorb onto their surface. This phenomenon of LSPR energy is called chemical interface damping (CID). The change in the dielectric constant of the surrounding medium due to organic molecule adsorption may result in LSPR peak shift, intensity variations, and linewidth change, which can be examined at the single-particle level. The AuNRs having biocompatible, photostable, and electrically conductive properties enable the possibility of combining spectroscopy with electrochemistry. Single-particle spectroelectrochemistry that combines single-particle dark field scattering-based (DFS) microscopy and spectroscopy with an electrochemical workstation made possible the electrochemical plasmonic sensing and tuning of the chemical interfaces at the single-particle level. AuNRs of the desired size (25 × 75 nm) were immobilized on indium tin oxide (ITO) substrates to construct plasmonic electrodes for this investigation. In this study, we discuss the CID effect induced by thiol molecule adsorption onto the AuNR surface. The effect of electrochemical manipulations at the bare AuNRs and the gold-thiol interface was examined. Electrochemical tuning of LSPR energy loss (or CID) at the interface of Au-thiol and its effects on the stability of thiol molecules on the Au surface was analyzed by probing the LSPR energy shift, change in peak intensity, and linewidth change for time-dependent and potential-dependent variations at the single-particle level.

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Analytical Chemistry

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Geographical Origin Discrimination of Soybean Paste Using Laser-Induced Breakdown Spectroscopy and k-Nearest Neighbors Analysis

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Laser-induced breakdown spectroscopy (LIBS) is one of the simple elemental analysis methods. The sample pre-processing is minimized, allowing the rapid analysis of most elements. In this study, we conducted discrimination of soybean paste based on its geographical origin using LIBS. Soybean paste is a seasoning widely used in East Asian countries. It is characterized by its high protein and amino acid content, excellent storage stability, and distinctive flavor and aroma, making it widely favored in culinary practices. In South Korea, numerous food companies distribute soybean paste products, with a significant portion being produced in China. Distinguishing the origin of soybean paste is crucial for food distribution management. A total of 167 soybean paste samples were used in this study, with 101 being domestically produced and 66 from China. LIBS equipment measurements revealed the presence of elements such as C, Mg, Na, K, H, Ca, Cl, and P in soybean paste samples. The interclass distance of these elements was calculated for each origin, and elements Mg, P, and C showed interclass distances exceeding 0.5. *k*-NN analysis was then conducted using these three elements, and the model incorporating Mg and C together demonstrated the highest accuracy. Therefore, the highest accuracy was achieved in the Mg-C model at k = 13, with 86.2%. Our research suggests that a discrimination method combining LIBS and *k*-NN can be an effective choice for determining the origin of soybean paste with a small number of samples, providing rapid results.

Poster Presentation : **ANAL.P-240**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Performance evaluation of thickness-tapered channel in flow field-flow fractionation with the effect of field programming in a uniform channel

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Flow field-flow fractionation (flow FFF) is a method employed for separating particulate materials based on particle sizes. Particles traverse a thin rectangular channel space with a carrier liquid, while crossflow, applied perpendicular to the channel axis, serves as the driving force for separation. To enhance the separation efficacy of flow FFF, field programming with a flow controller has been introduced, enabling varying crossflow rates over time to achieve lower retention times and improved separation performance. However, integrating a flow controller for field programming adds to the overall cost, prompting the need for a novel flow FFF technique capable of enhancing separation performance without altering flow rates.The introduction of a thickness-tapered channel in flow FFF presents a solution to this challenge, employing a channel with decreasing thickness along its length. This study directly compares the separation performance of the thickness-tapered channel with that of a conventional asymmetrical flow FFF channel using field programming. Results demonstrate that the thickness-tapered channel yields comparable separation performance to field programming, enhancing retention time and sample recovery.Continuing the evaluation, the thickness-tapered channel's performance will be assessed in the separation of lipoproteins. Enhanced resolution and sample recovery afforded by the thickness-tapered channel offer the potential for improved separation of low-density lipoproteins (LDL) and very-low-density lipoproteins (VLDL), which pose challenges in conventional flow FFF separations.

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Analytical Chemistry

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Top-down lipid analysis of exosomes derived DU145 cells using mAF4-ESI-MS/MS

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Extracellular vesicles (EVs) are cell-derived membrane-bound particles, including exosomes and microvesicles, characterized by a lipid bilayer structure. Exosomes (30–150 nm in diameter), which are released by the fusion of multivesicular bodies with the plasma membrane, play an important role in intercellular communication and are expected to serve as useful biomarkers for various diseases. Conventional lipidomic analysis of exosome lipids typically performed through bottom-up analysis using liquid chromatography-tandem mass spectrometry (LC-ESI-MS/MS). This method qualitatively and quantitatively analyzes total lipids by extracting the lipidome from biological sources with organic solvents. This study aims to demonstrate the potential of top-down analysis by miniaturized asymmetrical flow field-flow fractionation and electrospray ionization-tandem mass spectrometry (mAF4-ESI-MS/MS) as a high-speed screening platform for direct analysis of exosomes from the culture media of DU145 cells without extraction. Using an mAF4 channel, exosomes can be separated at high speeds (

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Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

SARS-CoV-2 induced lipid perturbation in lung, liver, and serum of mice

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The emergence of SARS-CoV-2, the virus responsible for COVID-19, has presented a significant danger to public health worldwide. COVID is characterized by symptoms such as tiredness, coughing, tightness in the chest, shortness of breath, palpitations, muscle pain, and difficulty with concentration. These symptoms may be associated with various conditions, such as damage to organs, syndrome following a viral infection, syndrome following critical care, and other related conditions. Lipids serve as both a source of energy and as essential components of cells, while also playing a crucial role in cellular signaling pathways and regulating the permeability of cell membranes. Therefore, metabolic alterations may result in changes in lipid composition and its level. In this study, the recovery process from the infection of COVID-19 will be observed in the lung, liver, and serum of K18-hACE2 mice by monitoring changes in lipid composition using nUHPLC-ESI-MS/MS. A total of 703, 869 and 466 lipids were identified in the lung, liver and serum samples from mice through qualitative analysis. At 1x10^2 PFU/mL (plaque forming unit), most lipid classes exhibited substantial decreases in lung tissue at 2 days post-infection (dpi), followed by subsequent recovery. Similarly, at 1x10^5 PFU/mL, most lipid classes showed significant reductions in lung tissue at 1 dpi, followed by subsequent recovery. However, TG (Triacylglycerol) showed a steady decreasing trend in lung tissue. Even in liver, most lipid classes decrease and then recover. Qualitative and quantitative analysis is being conducted to assess the degree of recovery in mice infected with COVID-19. This study will contribute to the understanding of organ damage and recovery resulting from COVID-19 infection.

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Optimization of skin sampling method for lipidomic analysis by nanoflow UHPLC-ESI-MS/MS

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The human skin serves as the primary physical barrier against the external environment, with the outermost epidermal layer, known as the stratum corneum, composed of lipids such as ceramides and glycerolipids. Tape stripping is a common method for skin sampling, involving the use of adhesive tape to collect stratum corneum layers. Due to various factors influencing lipid removal by each tape strip, a standardized sampling procedure is essential. This study aimed to optimize skin sampling method in terms of sampling location and the number of tape strips during repeated stripping. Skin samples were obtained from seven sequential tape strips taken from the same spot and from four different locations (forehead, forearm, cheek, and neck). Lipid analysis was followed by nanoflow ultrahigh performance liquid chromatography electrospray ionization tandem mass spectrometry (nUHPLC-ESI-MS/MS). Lipid profiles were analyzed by comparing the normalized peak area of individual lipid species relative to the peak area of internal standard specific to each lipid class. When skin samples were repeatedly taken from the same spot, the number of identified lipid species tended to decrease, which became significant after the 6th layer. To overcome the layer to layer variation in lipid composition, a pooling method of different tape strips was adopted. Extracts from the first 3 or 5 consecutive layers were pooled, respectively, and analyzed. This approach resulted in the identification of over 50 additional lipid species in the pooled samples compared to individual tape strip extracts. Prior to optimizing the number of tape strips for sample pooling, the variation in lipid composition and quantities among adjacent spots was evaluated. From statistical comparison of quantified results, the normalized peak area of each lipid species from the three adjacent spots were not statistically different from each other. Therefore, sample pooling was

adopted to establish the most representative tape stripping method that accurately reflects skin lipid composition and avoid loss of quantifiable lipids.

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Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Non-thiolated DNA-Templated Synthesis of Intra-nanogap for Highly Sensitive SERS Probes

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Plasmonic nanoparticles are increasingly recognized for their potential in biosensing applications, owing to their remarkable optical properties. Among these, plasmonic nanogaps, known as energetic ‘hot spots’, exhibit the ability to confine electromagnetic fields, resulting in strong Surface-Enhanced Raman Scattering (SERS) signals. This research endeavors to fabricate intra-plasmonic nanogap architectures utilizing non-thiolated DNAs, which offer a more cost-effective alternative to thiolated DNAs. We employed both salt-aging and low pH methodologies to modulate DNA grafting density, a crucial parameter in the formation of intra-nanogap structures within gold nanoparticles (AuNPs). The resultant intra-nanogap AuNP constructs demonstrate exceptional sensitivity in Raman signal enhancement, showcasing their potential as robust SERS-based biosensors.

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Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Lipid alternations in brain and spleen tissues of SARS-CoV-2 mouse using nanoflow UHPLC-ESI-MS/MS

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Various corona virus diseases including SARS and MERS, along with SARS-CoV-2, have been prevalent in the 21st century, posing ongoing concerns due to continuous mutation. Therefore, research is increasingly needed due to similarities in symptoms, infection, and metabolic pathways among betacoronaviruses.Lipids play a critical role in viral entry, replication, and assembly and are involved in many pathological symptoms. Hence, the accumulation of lipidomic research data can aid in early diagnosis and treatment strategies.To evaluate the impact of varying doses of SARS-CoV-2 on spleen and brain tissues over time, this study conducted qualitative and quantitative lipidomic analyses at six different time points. Mice were infected with two different levels of plaque-forming units (PFU), and their tissue lipids were analyzed in comparison to control group.In this study, we examined the lipid profiles of SARS-CoV-2-infected mice in both spleen and brain tissues using nanoflow ultrahigh-performance liquid chromatography-electrospray ionization-tandem mass spectrometry. Through this comprehensive non-targeted analysis, we identified a total of 593 and 926 lipids in the brain and spleen tissue, respectively. Remarkably, targeted quantification unveiled significant changes in the majority of lipids within the infected group, regardless of the infection dosage.Most of Phospholipids displayed a consistent decreasing trend in both brain spleen and brain tissues. On the other hand, sphingolipids (SLs) exhibited a notable increase in brain. But SLs show opposite trends in the spleen. Specifically, alterations were observed in the ratio between phosphatidylcholine and phosphatidylethanolamine, both prevalent in

cell membranes. Notably, this ratio exhibited a trend towards recovery beginning on the 7th day after infection. A thorough statistical analysis will be provided.

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Copolymerization of Regenerative Drugs in Biocompatible Microneedles to Maximize Drug Efficacy

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A regenerative drug, 1,4-dihydrophenonthrolin-4-one-3-carboxylic acid (1,4-DPCA), can inhibit the prolyl hydroxylase (PHD), which upregulates HIF-1α expression to induce cell regeneration under normoxia conditions. We developed a microneedle 1,4-DPCA loaded drug delivery system designed for target tissue regeneration. The reason for choosing microneedle-based drug delivery system is attributed to its advantages not only in targeted delivery, but in maintaining the appropriate concentration at the wounded site. To achieve this, we copolymerized vinyl functionalized 1,4-DPCA with the biocompatible monomer 1-vinyl-2-pyrrolidone (VP) triggered by UV irradiation. For the functionalization, diallylamine was chemically grafted to 1,4-DPCA through HBTU coupling reaction, resulting in covalent conjugation between VP and 1,4-DPCA. Our regenerative microneedle patch system offers a solution to overcome the low drug loading rates caused by the non-polar nature of 1,4-DPCA, by maintaining high drug loading efficiency and uniform drug release profile confirmed by HPLC analysis. Thus, we expected that the developed drug delivery system will be universally adopted for targeted tissue regeneration.

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Advanced 19F NMR Investigation of Poly (vinylidene fluoride) (PVDF) Crystalline Phases for Good-performance Electrode

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[1]*Department of Bio-Nano Engineering, Department of, Hanyang University, Korea*

With the growing demand and interest in lithium batteries in energy storage fields such as electric vehicles, smartphones, laptops, etc., research on binders, one of the important components of lithium batteries, has also increased. PVDF, known for its versatility as a dielectric polymer, exhibits four distinct crystalline phases: α, β, γ, and δ. Existing research has predominantly examined PVDF's binder efficacy through surface and electrochemical analyses, yet a comprehensive understanding of its behavior during battery cycling and the impact of its polymorphic nature remains underexplored.In this study, NMR analysis and IR analysis were conducted as an analysis method to determine the PVDF's crystallinity that affects battery performance.Initial phase of the research involved segregating commercial PVDF samples into their α and β phases via recrystallization techniques, and a series of 1H, 19F solution-state NMR experiments on the α and β films were conducted to delve into their structural and dynamic properties. Detailed structural properties of the PVDF materials were examined, however, phase information of the recrystallized phase was lost in the solution NMR measurements. To address this, solid-state 19F and 13C NMR experiments were conducted and phase transition issues of the PVDF were overcome in the advanced solid-state methodology. The outcomes of this research underscore the effectiveness of NMR-based method in accurately determining the intricate molecular structure and crystallinity of PVDF binders. These attributes have a direct and significant impact on the performance of electrodes in lithium-ion batteries, highlighting the crucial role of advanced material analysis in the progression of energy technologies.

Poster Presentation : **ANAL.P-248**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Advanced cross-polarization schemes for heteronuclear transfers involving labile protons in biomolecular solution NMR

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Heteronuclear 1H to 15N polarization transfers play a critical role in modern NMR techniques, especially in the study of biomolecules. These transfers can be achieved either through INEPT-based pulse sequences or J-driven cross-polarization (J-CP). INEPT is simpler, more reliable, and requires less power, but its effectiveness decreases with rapid chemical exchanges. Consequently, J-CP is often preferred for studying quickly exchanging labile protons, despite needing more power. Achieving effective J-CP relies on locking both HN and water protons along the same x-axis, allowing polarization transfer to continue even during exchanges. However, simultaneously locking labile and water protons while achieving a 1H to 15N Hartmann-Hahn J-CP match can be challenging, especially at high magnetic fields or when using cryogenically-cooled probes. This difficulty arises due to large chemical shift dispersions and limitations on the maximum achievable field strengths. This study introduces two new cross-polarization methods to overcome these challenges, enabling more effective double and triple resonance experiments with fast exchanging labile protons under physiological conditions.

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Analytical Chemistry

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Overcoming Undesired Autoxidation in Catecholic Polymers through a One-Step Phenol to Catechol Conversion Strategy

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We address the inherent limitation of catechol-containing polymers, which lose their original molecular adhesive properties due to self-crosslinking via oxidation in ambient environments. In this study, we introduce a one-step approach leveraging the Fenton reaction to facilitate a simple conversion from phenolic to catecholic polymers, effectively solve the issue of undesired spontaneous oxidation through providing catecholic polymer on demand. This strategy enables the polymers to be stored stably, significantly enhancing their applicability in various fields. The successful conversion of the polymer was spectroscopically confirmed through NMR and UV-VIS. To prove the successful catechol conversion, we conducted 180° peel tests and shear tests using UTM, which demonstrated improved adhesion and cohesion as noted in the previous study. Our research address the fundamental limitations of catechol-containing polymers; thus, it promises significant potential to influence the chemical design of relevant functional materials.

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Poster Presentation : **ANAL.P-250**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Harnessing Gallium-Based Nanoparticles for Environmental Remediation

Seoyoung Hur, Taesoo Cho, Jeong-Wook Oh*

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Gallium-based liquid metals have garnered significant attention for their unique properties, including low toxicity, high conductivity, and distinct UV absorption characteristics. Among these, eutectic gallium-indium (EGaIn) nanoparticles have emerged as a promising candidate for environmental remediation applications, particularly leveraging their potential in UV plasmonics. This study investigates the efficacy of EGaIn nanoparticles in degrading environmental pollutants under UV irradiation. By exploiting the UV absorption properties of EGaIn nanoparticles, we aim to enhance their performance in addressing environmental challenges. Through a series of experiments, we evaluate the ability of EGaIn nanoparticles to degrade various pollutants, shedding light on their potential as an effective tool for environmental cleanup.

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Poster Presentation : **ANAL.P-251**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Exploring EGaIn Nanoparticle Synthesis for Enhanced UV Plasmonic Applications

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Gallium-based liquid metals (LMs) have gained attention for their low toxicity, high conductivity, and low vapor pressure. Eutectic gallium-indium (EGaIn) nanoparticles, with unique UV absorption and surface activity, offer potential for UV plasmonics and molecular cleavage. Current synthesis methods, mainly sonication, struggle to achieve desired EGaIn nanoparticle morphology, yield, and size distribution. Tailoring EGaIn nanoparticle absorption requires adjusting morphology, chemical environment, and pH. We synthesized EGaIn nanoparticles under varied conditions (sonication parameters, solvent type, and pH) to study their impact on their morphology and size distribution. Our findings shed light on synthesis variables and suggest pathways for effective plasmonic applications.

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Poster Presentation : **ANAL.P-252**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of Thermogravimetric and Mass Analysis System

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With the advancement of the material industry, there is a need of simultaneous analysis for various characteristics of high-performance materials. Especially, in the case of materials that make up parts with important thermal stability, such as secondary batteries, it is particularly important to analyze the chemical composition of gas generated with changes of physical properties at high temperatures. The weight reduction of the sample analyzed through TGA is a major indicator of the thermal stability of the sample, which represents thermal properties such as thermal stability, life time and decomposition mechanism of the analyte. Qualitative and quantitative analysis of gas generated from each thermal decomposition process during TGA analysis can be performed by establishing the integrated system of TGA and TOF-MS. To this end, the integrated analysis instrument TGA TOF-MS was developed and applied to provide fundamental data for the development of advanced materials including thermal stability and chemical composition of evolved gas. Based on this, we can improve the product stability by analyzing the cause of thermal decomposition process.

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Poster Presentation : **ANAL.P-253**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Investigation on Raman spectral features according to variation of internal thickness of pearls

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Cultured pearls are produced by the secretions of shellfish that leading to form a thin film of artificial nuclei in the body and layers. Aragonite (calcium carbonate, $CaCO_3$) and conchiolin (protein) form a layer outside the nucleus, and are being stacked during the growth. This multi-layered structure, called the Nacre layer, determines the gloss and size of pearls, and is the factor that directly influences on the commercial value of pearl. However, it is difficult to estimate the internal thickness of the pearl layer, and only feasible when a pearl is cut for naked-eye examination. Therefore, a non-destructive analytical method for this purpose is critically required and Raman spectrscopy providing sensitive spectral information on the constituents of pearl is surely a candidate. Initially, the differences in the Raman spectra of Akoya pearls cultivated in the three countries (China, Japan, and Korea) were investigated. Next, since the Nacre layer is mostly composed of calcium carbonate, the intensities of corresponding peaks were examined and discussed in relation with the internal thickness of the Nacre layer.

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Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Urinary metabolic profiling in ECMO-treated severe COVID-19 patients

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Coronavirus (COVID-19) emerged in 2019 and continues to persist to this day. In severe cases of infected patients, extreme lung inflammation and damage may result in inadequate oxygen supply, necessitating extracorporeal membrane oxygenation (ECMO) therapy. In this study, we observed changes in urine metabolites following ECMO treatment, based on survival outcome and the presence of diabetes, using liquid chromatography tandem mass spectrometry (LC-MS/MS). We collected urine samples from 25 severe COVID-19 patients who received ECMO therapy in 2021 and 2022. These samples comprised 10 from deceased patients and 15 from survivors. Additionally, we categorized the samples based on the presence of diabetes, with 18 samples from non-diabetic patients and 7 from diabetic patients.As a result of multivariate analysis, partial least squares discriminant analysis (PLS-DA) score plots were generated using quantified 70 metabolites, showing separation based on survival and diabetes status. In metabolic profiling, elevated levels of ADMA, arginine, citrulline, folic acid, iso-carnitine, and nicotinamide were observed in deceased patients relative to survivors. And adenosine, ADMA, betaine, but-carnitine, folic acid, N-acetylglutamic acid, pyroglutamic acid, and TMAO were found to be elevated in diabetic patients compared to non-diabetic. These findings demonstrate the substantial metabolic alterations induced by COVID-19 infection. This study offers valuable insights of the utility of LC-MS/MS-based metabolomic analysis for observing urinary metabolites in severe COVID-19 patients.

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Poster Presentation : **ANAL.P-255**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Analysis of Ca in Urine Using Laser-Induced Breakdown Spectroscopy

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Urine analysis offers valuable insights into various bodily conditions, including abnormalities, diseases, and dietary imbalances. Notably, excessively high or low calcium levels may signal kidney disease, or other conditions. This study presents a novel approach to urine calcium analysis utilizing Laser-Induced Breakdown Spectroscopy (LIBS), renowned for its simplicity in sample preparation and rapid analysis. We prepared and analyzed 23 urine samples and NIST's SRM 2670. Given the challenges in obtaining ample biological samples, we adopted a focused approach using Laser-Patterned Silicon Wafer (LPSW) technology. Utilizing a grid pattern, carved by laser ablation, on a 1 cm x 1 cm silicon wafer surface and using plastic tape to minimize sample loss, 15 μL volumes of urine were deposited and dried. Measurements were conducted at 10,000 points within a 12 mm x 12 mm area, utilizing a commercial LIBS instrument (J200, Applied Spectra, Inc.) in a helium ambient gas. To generate the calibration curve, the concentrations were determined using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The calibration curve resulted in an R^2 value of 0.9248. Additionally, signal normalization using silicon (Si), a substrate component, further improved accuracy, yielding an R^2 value of 0.9650. To evaluate the calibration curve, the Leave One Sample Out (LOSO) method was utilized. The root mean square error (RMSE) was determined to be 54.5 ppm before normalization and 40.5 ppm after normalization. This innovative method of sample preparation and LIBS analysis using LPSW holds promise as a straightforward diagnostic tool for bodily fluid analysis, facilitating medical diagnosis in fields such as urine and blood analysis.

Poster Presentation : **ANAL.P-256**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Sex-specific reproductive dysfunction in zebrafish: Estrogenic and anti-androgenic effects of 4-tert-octylphenol

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Alkylphenols, such as nonylphenol and 4-tert-octylphenol (OP), are estrogenic chemicals generated through the breakdown of alkylphenol ethoxylates, posing risks to aquatic life and higher organisms. In this study, we examined OP's toxic influence on the reproductive hormones of both female and male zebrafish. For 21 days, the zebrafish were subjected to four OP concentrations (0, 20, 100, and 500 ng/mL), selected based on the minimum concentration (EC10 = 0.48 ng/mL) affecting zebrafish embryos. OP exposure led to a significant rise in liver vitellogenin mRNA levels and 17β-estradiol production in both genders. Conversely, OP's anti-androgenic impact was observed as a decrease in gonadal androgen receptor (AR) mRNA levels and a reduction in endogenous androgens (testosterone and 11-ketotestosterone) in males. Notably, cortisol and thyroid hormone concentrations increased with OP dosage in both sexes, influencing the regulation of gonadal steroids. Our data indicate that extended OP exposure results in persistent reproductive issues in adult zebrafish, largely due to the complex interactions between hormone levels and associated gene expressions. By conducting comprehensive biological response assessments in adult zebrafish, our findings offer essential insights into OP's reproductive toxicology, supporting further studies in aquatic environments.

Poster Presentation : **ANAL.P-257**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Lipidomic changes of brain tissue in an Alzheimer’s disease mouse model overexpressing Tau

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Alzheimer's disease(AD), the most common neurodegenerative brain disease that causes dementia, has been reported to have a steadily increasing incidence rate worldwide, but its therapeutics is not clearly defined. Abnormal accumulation of tau aggregates is considered a common pathological feature of Alzheimer's disease. However, research on the mechanisms underlying tau pathology associated with aberrant lipid metabolism within brain tissue are poorly understood.To evaluate the lipidomic changes in relation to Tau pathology, we performed lipidomic analysis of the brain tissues of PS19 wildtype mice aged 4.4-months and 11-months and human tau-overexpressing PS19 mice aged 4.4-months(early-stage AD) and 11-months (late-stage AD) using ultra performance liquid chromatography trapped ion mobility spectrometry time-of-flight mass spectrometry(UPLC TIMS-TOF MS). As a result of multivariate analysis, the score plot of principal component analysis showed a clear separation between the wild-type and Tau group at 11-month, stronger than at 4.4-month indicating significant alterations in the lipidomic profiles of the brain tissue from tau mice at 11-month. Specifically, in the late-stage tau group, the levels of cholesteryl ester, ceramide, triacylglycerol, and phosphatidylglycerol were significantly increased compared to the other groups.Therefore, our findings suggested that the alterations in lipid metabolism in the brain due to tau aggregation have a comparable between 4.4-month-old wildtype and early-stage AD, but reveal significant lipid accumulations as the disease progresses to late-stage AD. This study also demonstrated that lipidomic analysis using TIMS-TOF MS is a useful method to investigate lipid metabolism associated with Tau pathology and Alzheimer’s disease.

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Poster Presentation : **ANAL.P-258**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Metabolomics time-course response in liver tissues after SARS-CoV-2 infection

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[2] *Korea Basic Science Institute, Korea*

SARS-CoV-2 infects the nasopharynx and lungs, however, several studies have reported cases of acute liver injury and liver failure following SARS-CoV-2 infection. Moreover, changes in liver metabolism caused by SARS-CoV-2 have not been clearly identified. In this study, liver tissue was collected from hACE2 mice model (n = 57) intranasally infected with 10^2 Wuhan virus at 2, 5, 7, 14 days post-infection (dpi) and control group (no infection). Analysis of liver tissue from SARS-CoV-2 infection mice was performed by untargeted metabolomics approach using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF/MS). Clustering analysis based on 67 significantly changed hepatic metabolites after SARS-CoV-2 infection was performed to identify trends in metabolic changes in the liver, and three clusters were generated. In Cluster1, metabolite levels showed an increasing tendency after 2 and 5 dpi. In particular, significant changes could be observed in acyl-carnitines and amino acids levels, suggesting metabolic changes in response to early inflammation. Cluster2 displayed a rise in metabolite levels post 7 dpi. Notably, citrulline and dimethylglycine, elevated in severe coronavirus infection. Conversely, Cluster3 exhibited a tendency towards decreased metabolite levels in the infection group, with NAD+ gradually decreasing from 2 dpi to 14 dpi. This study demonstrated that hepatic metabolites has changed according on the time points during SARS-CoV-2, and LC/MS-based metabolomics may provide insight into metabolic pathway involved in liver dysfunction in SARS-CoV-2 infection.

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Poster Presentation : **ANAL.P-259**

Analytical Chemistry

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Streamlining LC-MS Sample Preparation: An Automated Robotic System Utilizing 3D Printing

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In this study, we developed an innovative robotic system to automate and simplify the sample preparation process for LC-MS analysis. Leveraging mature 3D printing technology, we utilized an open-source 3D printer to reduce development time and costs significantly.Manual sample preparation often encounters challenges such as inefficiency, lack of reproducibility, and difficulties in replication. To address these issues, we devised an automated sample preparation robot by integrating advanced 3D printing technologies. This involved adapting an open-source 3D printer, employing G-code language, implementing three-dimensional coordinate motion control kinematics, integrating a commercial 3D printer control board, and utilizing software like Klipper and web client for 3D printer management.Our system primarily targets the automation of preparation processes essential for LC-MS analysis, comprising three main subsystems: the Automated Liquid Handling System (ALHS), Automated Reagent Storage System (ARSS), and Automated Consumable and Equipment Storage System (ACESS).To evaluate the performance of our automated sample preparation robot system, we conducted a time-consuming TEMPO-free radical initiated peptide sequencing (TEMPO-FRIPS) peptide preparation process. Comparative analysis of time consumption and reproducibility of quantitative results was performed between manual and automated methods. To enhance accessibility and foster collaboration, all design files, manuals, and associated software of our system are provided as open-source resources, enabling researchers to freely utilize and customize them to improve the efficiency of their LC-MS analysis.

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Poster Presentation : **ANAL.P-260**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of a gas pre-treatment device for high-performance analysis

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In this study, we developed a new gas pretreatment device for moisture removal and constructed a system capable of remote operation via a web-based interface. As demonstrated by industrial accidents resulting in harmful gas leaks and the deterioration of air quality in urban areas, the precision of gas analysis is essential across various fields such as environmental monitoring, industrial process control, and health and safety management. Despite numerous advances in rapid and accurate gas analysis, prevailing methods often involve high costs and low user-friendliness. This research aims to overcome these limitations by developing a gas pretreatment device that effectively removes moisture, a common interferent in gas analysis. From a hardware perspective, we optimized gas injection by designing the internals using various valves and gas fittings. The moisture in the injected gas can be removed through a cooling-condensation process as it passes through a refrigerator module. On the software side, a system was built using Raspberry Pi and Arduino Mega to enable central control of the device, allowing users to remotely operate the device through a web-based user interface. The device will be used to pretreat gas samples, which will then be compared to untreated gas samples in terms of analysis efficiency. This comparison aims to validate the effectiveness of our pretreatment method in eliminating analytical interferents.

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Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

N-glycoproteome in prostate cancer tissues and blood for biomarker discovery

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Several diagnostic methods are being studied to increase the sensitivity and specificity of prostate cancer (PCa) diagnosis. The post-translational modification (PTM) pattern of protein is known to be a biomarker with much higher accuracy than the presence or absence and expression level of the protein in many diseases. Monitoring of alterations in glycosylation, which accounts for more than half of all PTMs, is evaluated to have potential in the biomarker field. This study intended to discover N-glycoforms related to PCa as biomarker candidates for more accurate early diagnosis. PCa tissues and blood samples were obtained from the same patients. Samples were prepared with methods developed in previous studies, and proteomes were identified through nLC-MS/MS analysis. N-glycoforms significantly found in PCa tissue and/or blood were shown by comparative analysis of identified proteomes.

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Poster Presentation : **ANAL.P-262**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Employing Multiple Regression to Analyze Factors Impacting Triboelectricity Output

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Triboelectric Nanogenerator (TENG) has been proposed to explore its versatile applications in human life, particularly its potential use in miniaturized devices. The operational principle of TENG revolves around contact electrification, a phenomenon wherein electric charges transfer from one material to another when they come into contact or are rubbed together. The output of triboelectricity is well known to significantly depend on the workfunction of each material involved. However it’s crucial to note that various variables, beyond just the work function, play a role in triboelectricity output. Understanding the intricate interplay of these factors is essential for optimizing triboelectricity output. To explore the influence of different factors, multiple regression analysis is employed to assess the significance of each variable. This statistical approach allows for a comprehensive examination of various factors and their impact on triboelectricity output.

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Poster Presentation : **ANAL.P-263**

Analytical Chemistry

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[Withdrawal] Advancing Antibody Sequences : TEMPO-based FRIPS Mass Spectrometry

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Poster Presentation : **ANAL.P-264**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of Sample Preparation Strategies of Formalin-Fixed, Paraffin-Embedded (FFPE) Tissue for Mass Spectrometry-based Proteomic Analysis

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Formalin-Fixed, Paraffin-Embedded (FFPE) samples are a type of tissue biopsy sample that can be stored at room temperature for a long time. Their stability facilitates the analysis of challenging-to-freeze tissues and enables the longitudinal tracking of disease progression. Recently, there has been a growing interest in FFPE proteomics, driven by the abundant availability of these preserved samples, which hold the potential to discover biomarkers for various diseases. However, analyzing FFPE samples presents challenges owing to chemical modifications in the samples induced by formaldehyde treatment. These modifications make it difficult to extract proteins and subsequent mass spectrometry (MS) analysis. In addition, there has been limited prior proteomic investigation of FFPE samples, unlike Fresh Frozen (FF) samples that are typically used in proteomics.This study aims to develop and compare two sample preparation protocols for mass spectrometry-based proteomic analysis of FFPE samples: in-solution digestion (ISD) and pressure cycling technology (PCT). The ISD method employs 2,2,2-trifluoroethanol (TFE) as a lysis buffer, ensuring effective protein denaturation and enhanced protein solubility. Meanwhile, PCT methods employ alternating high pressure to promote tissue lysis and enzymatic reactions, allowing for rapid sample preparation and high yield from a limited amount of sample. Proteomic data derived from the application of both methods to Mouse CRC Metastasis FFPE sections underwent comprehensive comparison, focusing on reproducibility, peptide yield, and quality of data.

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Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Human toxicity due to the combination of allethrin and DNA

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Allethrin, commonly used in mosquito repellents and pesticides, poses risks when exposed to sunlight due to the formation of hazardous decomposition products, as noted by the European Chemicals Agency. Exposure to sunlight leads to the breakdown of allethrin, predominantly yielding photolysis products containing epoxide structures. Epoxide compounds are implicated in the actions of chemical carcinogens, particularly in their ability to harm DNA. Hence, assessing DNA damage caused by allethrin is crucial, given that its photolysis product, containing an epoxide structure, has the potential to induce DNA damage. Photolytic products with allethrin m/z 169.09, 271.12, 319.19, 333.17, and 351.18 were identified in this study. Although binding to DNA was also tried, it was difficult to confirm with mass spectrum because there was too much salt, so the experiment is being optimized. In addition, confirming binding is challenging due to steric effects of DNA and allethrin's photo-degradation products. To address this, we will sequentially determine the presence or absence of binding to allethrin's photo-degradation products in the order of Nucleoside, Nucleotide, and DNA.

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Building a Miniature Digital Rectilinear Ion Trap Mass Spectrometer

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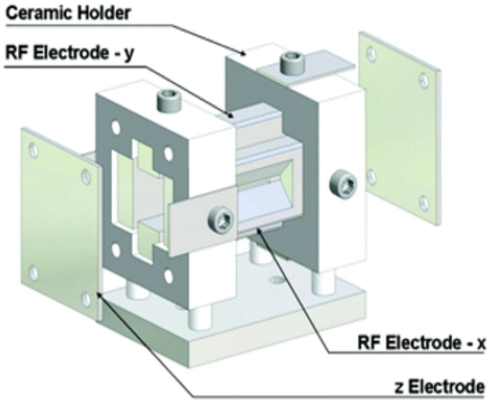
We aim to build a miniaturized digital rectilinear ion trap (DRIT) mass analyzer (10x10x40 mm^3) (Fig 1). Incorporation of digital technology in ion trap (Paul type, linear quadrupole) MS is not new. Recently, this got the most attention due to the advancement of digitization. We have already designed and manufactured the RIT based on the existing design of Ouyang et al. (Anal. Chem. 2004). These RITs have much simpler geometries than hyperbolic Paul traps, including higher trapping capabilities. A crucial advantage is the use of digital rectangular waveforms on the electrodes instead of classical rf-Sine waves. Besides, the mass scan is achieved by scanning the frequency while the voltage is held constant but not the opposite. Manipulation of the duty cycle of the trapping waveform and the excitation waveform allow to carry out mass (m/z) isolation and CID MS respectively without additional circuitry. In this contribution, we show simulation results of ion motions inside RIT employing commercially available software SIMION/SIMAX. Together with electrospray ionization (ESI) source, physical RIT assembly is tested using classical analog option where boundary ejection method is chosen successfully to generate the first mass spectra (Fig 1).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RF Electrode - y
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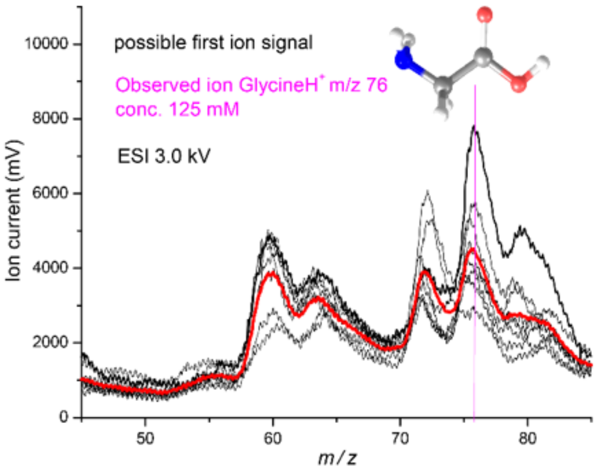
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Observed ion GlycineH+ m/z 76
conc. 125 mM
ESI 3.0 kV
Ion current (mV)
0
2000
4000
6000
8000
10000
50
60
70
80
m/z

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Poster Presentation : **ANAL.P-267**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Optimization of stainless-steel emitter fabrication methods to enhance sensitivity of electrospray ionization mass spectrometry (ESI-MS)

Somi Jeong, Hee-Ryung Kim, Sung Min Hwang, Hyunju Yang, Moonsu Bok, Sang-Won Lee*

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Emitter tips used in electrospray ionization are a crucial factor in effectively improving sensitivity of mass spectrometry. Etching, a method using the surface tension of liquid-solid contact, is one of the widely used principles in generating these tips. In our conventional method, fused silica capillary coated with polyimide is placed in a piranha solution to remove the coating which then the exposed glass is immersed in concentrated HF for chemical etching. However, it entails the possibility of an asymmetric taper from manual inspection and also involves chemical hazards due to the strong acidity of HF. To address these issues, we have modified the electrochemical etching method of stainless-steel needles proposed by Jansson et al., which uses a 1% diluted oxalic acid solution to reduce chemical hazards and ensure consistent taper. Moreover, stainless-steel emitters exhibit greater durability compared to fused silica emitters. To investigate the performance, proteomic data acquired with conventional fused silica chemical etched emitters and stainless-steel emitters generated from electrochemical etching was compared. The 5 W USB power adapter was replaced with a DC power supply which made precisely controlled electrochemical reactions possible using optimal parameters. The fabricated emitters were coupled with a home-built dual online liquid chromatography (DO-LC) system and an Orbitrap Exploris 480 mass spectrometer to analyze mass spectrometric data of enolase and HeLa digests. We concluded that with this modified method, sharp-tip emitters were produced allowing enhanced electrospray-ionization efficiency and sensitivity of mass spectrum.

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Wood inspired Reduced Graphene Oxide/Oxidized Carbon Nanotube/Polyvinylalcohol Aerogel for Efficient and Durable Solar Steam Generation

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Sustainable Nanochemistry Laboratory, Dongguk University, Korea
[1]*Department of Chemistry, Dongguk University, Korea*

Producing fresh water by purification or desalination with sunlight is a promising approach in the current water shortage situation. Graphene Oxide (GO)-based aerogel is widely utilized for solar steam generation (SSG) due to its low density allowing its floating, hydrophilicity and unique porous structure contributing to its high water absorption capacity. For efficient SSG, it is important to develop a GO-based aerogel that also features low density, high photothermal conversion, structural stability, vertical channels, and hydrophilicity. Herein, we present the development of GO-based aerogels consisting of polyvinylalcohol (PVA) and low-defect oxidized carbon nanotube (Ld-Ox-CNT) which meet the above-mentioned features. GO and Ld-Ox-CNT were synthesized with Brodie's method to introduce abundant hydroxyl groups for mimicking strong hydrogen bonding network between lignin and cellulose in a natural wood. Then, GO/Ld-Ox-CNT/PVA aerogel was fabricated by mixing individual components and freeze-casting, followed by lyophilization. After thermal treatment, the resulting thermally treated GO/Ld-Ox-CNT/PVA (T-GO/Ld-Ox-CNT/PVA) aerogel exhibited excellent mechanical strength, photothermal conversion, and water absorption properties. Under the 1 sun irradiation condition, the T-GO/Ld-Ox-CNT/PVA aerogel showed a high-rate evaporation (2.08 kg m^{-2} h^{-1}), efficiency, salt and pH tolerance. Additionally, it accomplished organic wastewater purification via SSG process while achieving continuous clean water production.

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Analytical Chemistry

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Thermal decomposition study of calcium oxalate hydrate through TGA and in situ FT-IR analysis

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In this study, the thermal behavior and molecular structure changes of calcium oxalate hydrate ($CaC_2O_4 \cdot H_2O$) were evaluated by using thermogravimetric analysis (TGA) and in situ fourier transform infrared spectroscopy (FT-IR), respectively. TGA was performed at a rate of 10 ℃/min from room temperature 25 ℃ to 1000 ℃ in air atmosphere. The temperature-dependent in situ FT-IR measurements were performed in combination with a high temperature reaction chamber (HVC) under ambient conditions. As a result of thermogravimetric analysis, a three-step decomposition process was observed at 150 ℃, 500 ℃ and 750 ℃ in the TGA curve of calcium oxalate. As a representative result, hydroxyl functional group peak of calcium oxalate hydrate disappeared in the FT-IR spectrum at 150 °C, which is consistent with the TG-DTA result. All hydrated forms of calcium oxalate hydrate (n = 1 ~3) will be included in future studies.

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Effective sample preparation for mass spectrometry-based bottom-up proteomics

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Proteomics is an increasingly utilized approach to gain insights into biological systems. However, the primary obstacles in proteomic analysis is the lengthy low reproducibility and potential for sample loss and contamination caused by multi-step sample preparation. This study aims to establish effective sample preparation for mass spectrometry-based bottom-up proteomics by comparing and validating three different trypsin digestion methods. the traditional overnight digestion, rapid digestion, and digestion using spin column methods. Proteins from commercial available serum were prepared with triplicates for each method and each sample was analyzed twice by tandem mass spectrometer equipped with liquid chromatography. First, the digestion efficiency of three methods was compared, calculated based on digested peptides from proteins extracted in urea-based lysis buffer. Second, the quality of identified results was examined by the number of peptides and proteins, the distribution of Xcorr value of identified peptides, the number of missed cleavage peptides, non-tryptic peptides and oxidized peptide and the sequence coverage of proteins. Third, the quality of quantified data was evaluated by the number of quantified proteins, the CV% of proteins quantified from LC-MS/MS duplicates, the distribution of coefficient of variation from intra-sample preparation (triplicates) across three sample preparation methods. Traditional method requires the longest time (over 16 hr) but incurs the lowest cost. In contrast, the rapid trypsin and digestion spin method can save the time, reducing enzyme incubation to less than

one hour but at a cost more than 1.5 times that of the traditional method. We should select the best methodological sample process based on the specific research needs to advance our understanding of complex biological systems and improve proteomic precision are required. Ultimately, this contributes to acquiring the reproducible and accuracy results in proteomics and marking a stride towards more reliable and insightful biological discovery.

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Poster Presentation : **ANAL.P-271**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Advancing Analytical Strategies for the Comprehensive Detection and Quantification of Cyclic Imines in Marine Ecosystems

Hyewon Kim, Hyun Joo An*

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Rapid changes in the marine ecosystem have brought attention to emerging toxins such as Cyclic Imines (CIs), posing a significant risk. Indeed, cases of exposure to the risk of CI toxicity are continuously reported in various European countries, but the absences of established international standards hinders effective management. CI analysis present challenges due to the limited availability of commercial standards (only seven out of more than 40 reported analogues) and their presence at very low concentrations in marine organisms along with numerous interfering lipophilic substances. In this study, we developed a multi-step platform to simultaneously identify and quantify CI analogs encompassing extraction, purification, analysis, and data interpretation. In particular, the development of an in-silico library capable of predicting elution time and MS/MS pattern is noteworthy. This predictive capability is based on the commercialized CI series including 3 types SPX, 1 type GYM, and 3 types PnTX. Using this platform, we successfully monitored CI isomers in approximately 400 species of shellfish collected from the Korean Peninsula over a span of 4 years. Note that PnTX G (4.131~14.42 pg/g), GYM A (21.23~309.9 pg/g), and 13-desMe SPX C (4.502~15.19 pg/g) were detected for the first time in about 110 species. Detected CI concentrations exhibited a positive correlation with increasing sea surface temperature. By applying this innovative analysis platform in real-world marine ecosystems, our approach holds promise for the ongoing monitoring and safety management of marine biological toxins.

Poster Presentation : **ANAL.P-272**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Characterization of self-assembled micelle inhibitory RNA drug using ion-pairing reversed-phase liquid chromatography combined with mass spectrometry

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Oligonucleotide drugs are promising therapeutics for various diseases, driving significant research efforts towards their development and enhancement. The conventional siRNA drugs have limitations in delivery efficiency, to address this, SAMiRNA, which combines hydrophilic and hydrophobic groups at both ends of the sense strand, has been developed. Given the heavy chemical modifications in SAMiRNA, its behavior in ion-pairing reversed-phase liquid chromatography (IP RPLC) combined with mass spectrometry (MS) is expected to differ from that of conventional siRNA drugs. Therefore, the development of appropriate analytical methods is warranted. The composition of ion pairing reagent in the buffer system directly affects chromatographic separation and sensitivity of detection by ultraviolet spectrometer and mass spectrometer. This study investigates various ion pairing reagents' effects on oligonucleotide LC systems and enhances method reliability through reproducibility experiments. Dibutylamine, paired with 1,1,1,1,3,3,3-hexafluoro-2-propanol, was employed, with separation on a C18 column, and LC-MS spectra were obtained using a Q-Exactive Plus mass spectrometer. In addition, SAMiRNA was analyzed at seven different column temperatures to observe the duplex form. Below 40 ^{o}C, the duplex peak was detected. Simultaneously, at the retention time of the duplex, antisense and sense strand peaks were observed. The behavior of the SAMiRNA duplex form more closely resembled that of the sense strand than the antisense, likely due to the presence of hydrophilic and hydrophobic groups at both ends of the sense strand.

Poster Presentation : **ANAL.P-273**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Metabolic Isotope Labeling of Glycans in C. elegans for Quantitative Glycomics by Mass Spectrometry

Jin-il Kim

Department of Chemistry, Changawon National University, Korea

N-glycosylation is one of the most important post-translation modifications. Glycans formed through it can affect biochemical properties and physiological functions of in vivo. In order to decode the correlation of glycan’s prevalence with their physiological contribution, many mass spectrometry (MS) with stable isotope labeling-based methods have been developed for the relative quantification of glycans. Based on the MILPIG (metabolic isotope labeling of polysaccharides with isotopic glucose), we establish an isotope labeling method and extend the quantitative glycomics using C. elegans as the model system.In order to apply the MILPIG strategy to the C. elegans model, a holidic medium capable of controlling glucose concentration was prepared in a glucose-free medium without E. coil and cornmeal, which cannot control glucose concentration. C. elegans was grown in a glucose concentration-controlled medium, and after purification of the glycans, the mass spectrum of C. elegan’s glycans was obtained by mass spectrometry. Additionally, the mass spectrum of isotopically labeled glycans was obtained in a medium containing isotopically labeled glucose (1-13C1) instead of normal glucose. Quantitative information was provided through comparison of the area of isotope clusters in mass spectrum from the same amount of normal and isotopically labeled glycans.

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Poster Presentation : **ANAL.P-274**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Photo-reversible tuning of chemical interface damping in single gold-nanorods with cucurbit[n]uril and aminoazobenzene

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Department of Chemistry, University of Ulsan, Korea

Photoresponsive molecules are well known as photoswitches because of their reversible changes in structural, electrical, and optical properties in response to photon stimulation. Among the photoresponsive molecules, azobenzene is characterized by photoisomerization, which changes from trans to cis form under UV irradiation. This photoisomerization of azobenzene has been widely studied to develop novel nanoswitches and electronic devices in combination with plasmonic nanoparticles. In this study, we have measured the chemical interface damping of gold nanoparticles due to the photoreactivity of azobenzene molecules upon attachment of cucurbit[n]uril hydrate molecules accepting aminoazobenzene to the surface of single gold nanorods. Among the various cucurbit[n]urils, we used cucurbit[6], cucurbit[7], and cucurbit[8], which have sufficient cavities to accommodate aminoazobenzene molecules. We found that aminoazobenzene generally leads to a greater damping effect of gold nanoparticle attachment in the trans form, but the aminoazobenzene cavity-accommodated in cucurbit[n]uril has more damping effect in the cis form. This work will provide insight into understanding how aminoazobenzene acceptance in supramolecules such as cucurbit[n]uril affects photoreversible molecular reactions.

Poster Presentation : **ANAL.P-275**
Analytical Chemistry
Exhibition Hall 2 THU 11:00~13:00

Metabolic Isotope Labeling of O-linked Glycans using Isotope-labeled Glucose in Yeast for Quantitative Glycomics

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The post-translational modification (PTM) process of proteins plays a critical role in their function and activity. O-glycosylation is one of the PTM process in which sugar molecules attach to oxygen atoms of the serine/threonine residues of proteins. During glycosylation, glycans attached to affected proteins are modified compared to normal proteins. Therefore, it helps diagnose diseases, so it can be used as a biomarker for diseases such as cancer and Alzheimer's. Glycans are a type of complex carbohydrate composed of glycoprotein components and play an important role in determining the biological activity and function of glycoproteins. To decipher the correlation between prevalence and physiological contribution of glycans, many mass spectrometry and stable isotope labeling-based methods have been developed for relative quantification of glycans. Among them, Metabolic Labeling of Glycans Using Isotopic Glucose for Quantitative Glycomics (MILPIG) is an in vivo labeling method that can produce isotope-labeled isotope glycans using isotope glucose (1,2-^{13}C2 glucose) as a carbon source. In this study, we extend quantitative glycosmics by applying MILPIG to yeast for baking. Yeasts were cultured in medium with normal glucose and in 1,2-^{13}C2 isotope-labeled medium, respectively, and mass spectra were obtained after glycan purification.Unlike conventional MILPIG, which used 1-^{13}C1 glucose to produce a mass difference of 1 Da per unit, 1,2-^{13}C2 glucose results in a mass difference of 2 Da per unit per unit, minimizing the overlap of the spectrum. Quantitative information was obtained by comparing the peak areas of the mass spectra in equal amounts of glycans.

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Poster Presentation : **ANAL.P-276**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of a Custom-Built Parahydrogen Injection System for Studying the Radical Scavenging Mechanism of Nicotinamide Derivatives

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Nicotinamide derivatives, such as nicotinamide adenine dinucleotide (NAD) and nicotinamide adenine dinucleotide phosphate (NADP), play crucial roles in various biological processes due to their involvement in redox reactions and energy metabolism. One of the significant advantages of nicotinamide derivatives in biological applications is their ability to act as radical scavengers. However, the mechanism underlying this behavior is raveling. Here, we investigate a radical scavenging mechanism using nicotinic acid hydrazide (NAH) with a custom-built parahydrogen injection system. We utilized the Arduino microcontroller to control the injection time using high nitrogen gas pressure. To monitor the reaction, we optimized the short injection time by several seconds; therefore, we obtained the reaction rate and time dependence spectra to unravel the radical scavenging mechanism using NAH.

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Poster Presentation : **ANAL.P-277**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Electrochemical Impedance Spectroscopy Analysis for Non-destructive Determination of Compressive Strength of Concretes

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To date, methods used to assess the interfacial transition zone (ITZ), which represents the boundary between the aggregate and paste inside concretes, have primarily relied ondestructive tests, and non-destructive tests has received little attention until recently. This study assessed the interfaces of concretes with lightweight aggregates based on electrochemical impedance spectroscopy (EIS) for high-strength concretes and examined the possibility of estimating the compressive strength of concretes through non-destructive testing using EIS. The experimental results revealed that the impedance of the hardened cement increased with increasing compressive strength and aggregate density. In particular, when the results of impedance measurement were displayed as a Nyquist plot, the intercept of the x-axis depicting the effective conductivity was proportional to the compressive strength. Furthermore, an equivalent circuit was selected to interpret the correlation between cement aggregates and impedance. Consequently, the compressive strength was found to increase with the value of the resistances of the electrolyte filled in continuous pores in the cement aggregate. And, the pores formed in the ITZ affect this value. The resistance at the ITZ for different aggregates was also obtained, and it was found that the resistance was consistent with the results predicted by SEM images of the ITZ and correlated with the strength of the concretes. The proposed method can be used as a way to easily determine the strength of cement according to differences in aggregate.

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Poster Presentation : **ANAL.P-278**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Comprehensive Characterization of Brain Gangliosides from Alzheimer’s Disease Mouse Model using Chromatographic Separation and Tandem Spectral Library Matching

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Gangliosides, which make up less than 1% of the total brain, are important components involved in nerve growth and development, neurotransmitter transport, and prevention of cell death. Recent research has notably focused on the potential of gangliosides in the diagnosis, treatment, and prevention of brain-related disease such as Alzheimer's disease (AD). However, the analysis of gangliosides is challenging due to their complex structure, characterized by a ceramide lipid tail and a glycan head group.. Here, we developed an LC/MS-based platform for the comprehensive characterization of brain gangliosides and observed changes associated with AD. First, we efficiently isolated complex gangliosides from brain tissue using a C18 column, which is mainly influenced by lipid composition. Then, structure-specific b-/y-ions such as m/z 454 ([Hex+Neu5Ac+H]+), 583 ([2Neu5Ac+H]+) and 657 ([Hex+HexNAc+Neu5Ac+H]+) were monitored to assign isomers with different positions of the terminal sialic acid. Our LC/MS-based data interpretation strategies enabled the comprehensive characterization of gangliosides through the integration of structure-based MS/MS spectra and RT predictions. To facilitate interpretation, we utilized the Personal Compound Database and Library program to construct a meticulously curated database, systematically cataloging compound details such as formula, exact mass, and RT. Indeed, we successfully characterized 79 ganglioside compounds extracted from representative five regions in AD model and normal mouse brain. Furthermore, the identification and quantitative comparison of isomers such as GD1a/b allowed for the prediction of ganglioside synthetic pathways. This analysis revealed significant changes in major gangliosides, including GT1b in the hippocampus,

comparing changes across the olfactory bulb, hippocampus, cortex, thalamus, and cerebellum, revealing. Our strategies offer a valuable reference for LC-MS-based ganglioside studies, facilitating comprehensive analysis and understanding in various biological samples.

Poster Presentation : **ANAL.P-279**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Structural study for APP-TM ion channel using NMR Spectroscopy

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The Amyloid-beta precursor protein (APP) is a membrane protein highly concentrated within neuronal synapses, acting as a cell surface receptor and implicated in various functions including synapse formation, neural plasticity, antimicrobial activity, and iron export. Amyloid beta (Aβ), generated through a distinct cleavage pathway of APP in the brain, is strongly associated with neurodegenerative diseases, notably Alzheimer's, owing to its propensity for oligomerization. One proposed mechanism of Aβ toxicity involves the formation of ion channel pores in neuronal membranes, disrupting cellular Ca2+ homeostasis. Numerous inhibitors targeting these ion channels have been explored, focusing on structural features influencing interactions with amino acids and inhibitor functional groups. Zinc (II) ions, abundant in nerve cells, are among the investigated blockers. This study concentrates on a human APP fragment encompassing amino acids 692-723th within the transmembrane domain (hAPP-TM), known for its zinc ion affinity. Solution-state NMR is employed to elucidate residue interactions of hAPP-TM with zinc (II) ions via chemical shift perturbation analysis. Additionally, solid-state NMR is employed to investigate the protein's structural dynamics and orientation in bicelle environments.

Poster Presentation : **ANAL.P-280**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

NMR-based structural analysis of anti-inflammatory peptides, tIK series

Jujin Park, Minseon Kim, Yongae Kim*

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Rheumatoid arthritis, an autoimmune condition, induces inflammation in the synovial membrane surrounding joints, leading to the degradation of ligaments and cartilage. This disease is believed to arise from an imbalance between pro-inflammatory and anti-inflammatory cytokines. Prior investigations have demonstrated that the inhibitor protein K562 (IK) suppresses the expression of pro-inflammatory cytokines. Similarly, the truncated IK (tIK) protein, comprising a specific region of the IK protein, exhibits similar inhibitory effects.However, the molecular weight of the tIK protein (29 kDa) poses challenges for its application in pharmaceutical processes. Consequently, we designed novel peptides derived from the tIK protein to maintain its anti-inflammatory properties while featuring shorter sequences. This led to the development of tIK-9mer, 14mer, and 18mer peptides (collectively the tIK series), which showed potent anti-inflammatory activity in preclinical trials. Further in-depth structural analysis is imperative to elucidate their mechanisms of action and optimize their therapeutic potential.The structural examination of tIK involved several critical steps employing NMR spectroscopy. Initially, we utilized DNA recombinant *E. coli* to express the tIK series. Subsequently, highly pure peptides were obtained through an optimized isolation and purification procedure. The molecular weight and purity were confirmed using MALDI-TOF mass spectrometry. Employing spectroscopic techniques such as NMR and CD, we analyzed the secondary structure of the peptides. Resonance assignments for individual amino acid residues were established via one- and two-dimensional NMR experiments.

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Poster Presentation : **ANAL.P-281**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Elucidative structure of m-hMC4R-TM2 and wt-hMC4R-TM2 using NMR

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Melanocortin receptors (MCR) are members of the rhodopsin family included in 7-transmembrane G protein-coupled receptors (GPCR). Five human melanocortin receptors (hMCRs) mediate the diverse actions of these melanocortin. Among them, the human melanocortin-4 receptor (hMC4R) is primarily expressed in the central nervous system so it is referred to as the neural MCRs which regulates metabolism. Mutations of MC4R are the most common monogenic form of obesity. Between many mutations, we focused on aspartic acid substituted with asparagine, located in the 90th amino acid in the second transmembrane domain (TM2). Since the structural difference between wild type-hMC4R-TM2 (wt-hMC4R-TM2) and mutant-hMC4R-TM2 (m-hMC4R-TM2) is expected to cause functional loss, we studied the structure of the target proteins.To analyze the structure of the proteins, we obtained pure protein using Fast Protein Liquid Chromatography (FPLC) using a size exclusion column. During the purification process, we used SDS as a detergent because the target proteins were hydrophobic. However, SDS was removed after FPLC to obtain high-purity proteins. This ensures that structural elucidation is not interfered with due to strong binding of SDS to target proteins. Therefore, a method of removing SDS was used to obtain high quality of pure protein. And the removal of SDS from the target protein was confirmed through MALDI-TOF. We performed various spectroscopy techniques such as CD spectroscopy, solution-state NMR spectroscopy, and solid-state NMR spectroscopy to confirm the structure.

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Poster Presentation : **ANAL.P-282**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

NMR Analysis of LPcin, an antimicrobial peptide, and Metal ion

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Antimicrobial peptides (AMPs) are an essential part of the innate immune system present in a variety of organisms. Unlike the mechanism of action of existing antibiotics, AMP interacts with the lipid membrane of microorganisms and then penetrates the membrane, ultimately kills the microorganisms. Since most AMPs have the form of an α-helix, they enter lipid membranes and play an important role in destroying lipid membrane. Additionally, it can effectively attach to the lipid membranes of bacteria because they have cationic amphipathic properties. Many of these cationic AMPs have excellent antimicrobial activity on their own, and it is known that the presence of additional divalent ions often improves the antimicrobial activity of AMP. In this study, we sought to investigate the correlation between LPcin analogs designed based on the structure of LPcin, a cationic antimicrobial peptide derived from bovine milk, and the divalent ions copper(II) and zinc(II). The structural stability of LPcin analogs in the presence of divalent ions was studied using various analysis techniques, and the degree of inhibition for various bacterial species was confirmed through antimicrobial activity experiments. These results suggest that the presence of divalent ions contributes to some extent to the structural stability and antimicrobial activity of LPcin analogs.

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Poster Presentation : **ANAL.P-283**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Studies of Syndecan-4 and PIP_2 in signal transduction by NMR spectroscopy

Yewon Lee, Minseon Kim, Yongae Kim*

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Syndecan is a membrane Heparan sulfate proteoglycan (HSPG) which consists of core protein and heparan sulfate. It is found at the cell surface and in the extracellular matrix, where it interacts with a variety of ligands, and performs the functions of cell-to-cell interaction, and growth-factor-receptor-activation. Syndecan-4, a member of the Syndecan family, is expressed in most mammal cells and participates in several signal transduction pathways, and for this PIP_2 binds to the V region of cytodomain. The binding of the ligand activates PKCα and induces the Syndecan-4 oligomer, in which the GXXXG motif of the transmembrane domain plays an important role in dimerization. Thus, this amino acid sequence was replaced and its effect on the formation of the oligomerization structure of Syndecan-4 was investigated.To obtain Syndecan-4 in large quantities and conduct NMR structural studies, genetic recombination techniques were used, and MALDI-TOF mass spectroscopy, CD spectroscopy, and solution/solid-state NMR were conducted for structural studies of the expressed protein. In addition, the interaction between the two molecules of PIP_2 and Syndecan-4 was investigated through 2D solution-state NMR experiments since it is important to investigate its structure to better understand the function and mechanism of Syndecan-4.

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Poster Presentation : **ANAL.P-284**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Spatiotemporal Dynamics of Real-time Catalytic Activity on Plasmonic Gold Nanoparticles at Resolutions Beyond the Diffraction Limit

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A one-shot dual-detection-based single-molecule super-resolution imaging method has been developed to observe the catalytic activity on the surface of individual plasmonic gold nanoparticles in real-time, aiming to understand the spatiotemporal dynamics of surface properties. This method simultaneously measures the scattering intensity on the gold nanoparticle surface and the fluorescence of resorufin molecules, enabling an investigation of the relationship between nanoparticles and catalytic reactions at the single-molecule level. Chemisorbed adsorbates induce changes in the electron density of individual gold nanoparticles throughout the catalytic cycle, causing fluctuations in the scattering intensity of individual nanoparticles. This phenomenon is attributed to electron transfer between reactant resazurin molecules and gold nanoparticles. The increase in the electron density of individual nanoparticles influences the catalytic reaction rate. Additionally, sequential mapping of individual catalytic events at sub-diffraction limit resolution has been achieved, providing real-time insights into the surface dynamics and spatiotemporal activity variations on the single gold nanoparticle surface. This developed method holds the potential to advance the development of heterogeneous catalysts based on nanoparticles at resolutions beyond the diffraction limit.

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Poster Presentation : **ANAL.P-285**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

Analyzing Stomach Cancer Tissue using Hyperspectral imaging and deep learning model

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Autofluorescence is a non-invasive analysis method which is used to diagnosing for in vivo and ex vivo tissues. Normally, Autofluorescence appears at a wavelength of 400 nm to 700nm and includes various biometric information. Among them NADH and FAD are co-enzymes used in metabolism and respirations, which are strongly associated with pathological symptoms. In addition, various components such as Lipofuscin PPIX and vitamins show fluorescence, and the change in composition appears as a change in fluorescence spectrum. In this study, we acquired centimeter-scale hyperspectral fluorescence images of tissue sections using a whisk broom method. Subsequently, we conducted semantic segmentation using a deep learning model, specifically a 3D Convolutional Neural Networks model. Hyperspectral imaging, a multi-channel imaging technique incorporating spatial and spectral information, facilitates detailed analysis of tissue characteristics at a microscopic level, and a 3D CNN model was employed to analyze and classify the spatial correlations within these images, with the categorized data being subsequently visualized and validated through Hematoxylin and Eosin (H&E) stained images.Since the CNN model can recognize patterns in the image and identify objects, achieving high-accuracy analysis becomes possible when combined with a hyperspectral image. Utilizing this method, we segmented the tissue into five types - mucosa, submucosa, muscle, muscularis mucosa and cancer, which showed high similarity with the results from pathological analysis.

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Poster Presentation : **ANAL.P-286**

Analytical Chemistry

Exhibition Hall 2 THU 11:00~13:00

ANALYSIS OF AIRBORNE DISINFECTANT RESIDUES AND EXPOSURE INVESTIGATIONSion Lee 1, Eun Woo Choi 1, Han bin Oh *11Department of Chemistry, Sogang University, 35, Baekbeom-ro, Mapo-gu, Seoul, 04107, Korea

Sion Lee

Chemistry, Sogang University, Korea

The COVID-19 pandemic has prompted a significant global increase in the use of disinfectants for sanitation purposes. This trend raises the potential concerns regarding the long-term harmful effects of disinfectants on human health. Evaluating the effects of disinfectants on human health requires a comprehensive approach beyond merely providing exposure concentration data. It necessitates consideration of factors such as changes in residual substances concentrations over time and substance capture potential.In this study, quaternary ammonium compounds (QACs, specifically alkyldimethylbenzyl ammonium chloride) were sprayed at a concentration of 500 ppm for 4 minutes within a space of 105 m3 using either automatic or manual spraying method. Airborne QACs were collected by drawing air at a flow rate of 1.5 L/min using an air pump, with a sampler containing a glass fiber filter serving as an adsorbent installed in the suction path. This design allowed the attachment of QACs to the glass fiber filter during indoor air drawing. Quantitative analysis of all samples was performed using LC-ESI-SRM/MS.The cumulative capture of QACs exhibited a sigmoidal function trend as a function of the capture time. For QACs sprayed via the automatic method, the maximum cumulative capture was 8.21 μg at the fromt and 1.36 μg at the back. Conversely, in the case of the manual method, the maximum cumulative captures were 0.14 μg at the front and 0.29 μg at the back. Notably, the sprayed QAC rapidly descended to the bottom of the room immediately following the cessation of spraying, thereby limiting the quantity of airborne QACs. The ratio of airborne QACs was determined to be 0.31 – 0.50 fo automatic spraying and 0.005 – 0.014 for manual spraying. In summary, the study demonstrates that the concentration of airborne QACs remaining in the air 10 minutes after spraying was minimal, also limiting health hazard.

Poster Presentation : **LIFE.P-126**

Life Chemistry

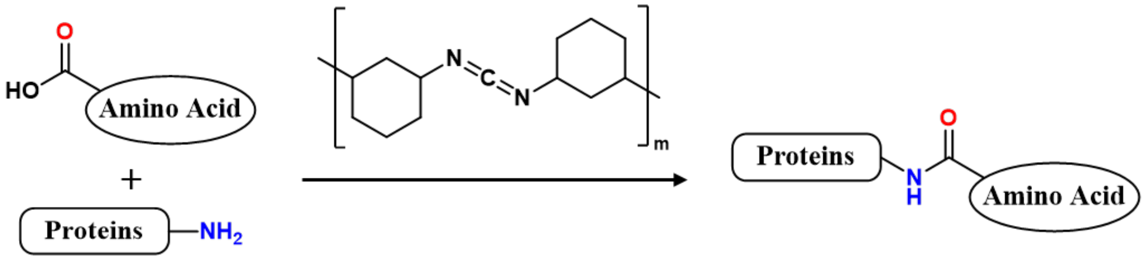
Exhibition Hall 2 FRI 11:00~13:00

Determination of pore inside hair fibers and carbodiimide reaction for damage repair

Hyun sub Park

R&D Center, LG Household & Health Care Ltd., Korea

The structure of hair can be broadly divided into three parts: the outermost layer called cuticle, the cortex that forms the bulk of the hair, and the innermost core known as medulla. The medulla is not present in all hair types and it has relatively less importance and research focus due to its smaller contribution to overall hair properties. The medulla is located inside the hair but is sensitive to various damaging factors and has a structure that is prone to damage. One common phenomenon that occurs when the medulla is damaged is the formation of pores. Hair with pores has lower tensile strength, elasticity, and luster compared to hair without pores. The luster of the hair is not only determined by the condition of the hair surface (cuticle) but also by the light reflected within the hair. In hair with a high internal density, reflection occurs well, but in the case of hair with pores, the amount of light reflected decreases due to scattering, resulting in a decrease in luster. In this study, we aim to introduce a method for non-destructive observation of the internal pore within hair fiber using an optical microscope, and present the results by representing the hair's internal density. We conducted a study on the tendency of hair's internal pore to increase due to the use of surfactants, which are the cause of damage. We coupled amino acids to the internal proteins of the hair using DCC coupling and confirmed the effects of increased internal density and increased luster as a result.



HO
O
Amino Acid
+
Proteins
NH2
N
C
N
m
Proteins
N
H
O
Amino Acid

Poster Presentation : **LIFE.P-127**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

21 Fluorescent Protein-Based DNA Staining Dyes

Yurie Kim, Kyubong Jo[1,*]

chemistry, Sogang University, United States

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Fluorescent protein–DNA-binding peptides or proteins (FP-DBP) are a powerful means to stain and visualize large DNA molecules on a fluorescence microscope. We constructed 21 kinds of FP-DBPs using various colors of fluorescent proteins and two DNA-binding motifs. From the database of fluorescent proteins (FPbase.org), we chose bright FPs, such as RRvT, tdTomato, mNeonGreen, mClover3, YPet, and mScarlet, which are four to eight times brighter than the original wild-type GFP. Additionally, we chose other FPs, such as mOrange2, Emerald, mTurquoise2, mStrawberry, and mCherry, for variations in emitting wavelengths. For DNA-binding motifs, we used HMG (high mobility group) as an 11-mer peptide or a 36 kDa tTALE (truncated transcription activator-like effector). Using 21 FP-DBPs, we attempted to stain DNA molecules and then analyzed fluorescence intensities. Most FP-DBPs successfully visualized DNA molecules. Even with the same DNA-binding motif, the order of FP and DBP affected DNA staining in terms of brightness and DNA stretching. The DNA staining pattern by FP-DBPs was also affected by the FP types. The data from 21 FP-DBPs provided a guideline to develop novel DNA-binding fluorescent proteins.

Poster Presentation : **LIFE.P-128**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Cell-Free Protein Expression System in a Single Liposome to Create Artificial Cells with Energy Harvesting Capabilities

Seangly Tror, Huong Thanh Nguyen[1], Kwanwoo Shin[2,*]

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Cell-free protein expression (CFPE) has garnered significant attention in biotechnology in recent years, as it enables high-throughput cloning with mRNA extracted from cells in an in vitro environment devoid of cells or microorganisms. This CFPE system, on the other hand, can be applied for protein production within artificially created liposomal spaces, representing a pivotal technology for understanding cellular metabolism and realizing regenerative artificial cells. In this context, our objective was to synthesize proteorhodopsin (PR), an energy-harvesting protein, through cell-free expression to create an artificial cell capable of generating its own energy within the liposomal space. We confirmed that our system successfully synthesized the PR protein within a single liposome and induced its translocation to the phospholipid membrane, demonstrating the viability of this approach. This study will further present the function and properties of the synthesized PR, elucidate the mechanism of cell membrane translocation, and provide optimization results. The cell-free protein expression model in a single liposome has the potential to evolve into an artificial eukaryotic cell-like model with comparable biological properties, including transcription and translation, as well as metabolic functions similar to natural cells.Cell-free protein expression (CFPE) has garnered significant attention in biotechnology in recent years, as it enables high-throughput cloning with mRNA extracted from cells in an in vitro environment devoid of cells or microorganisms. This CFPE system, on the other hand, can be applied for protein production within artificially created liposomal spaces, representing a pivotal technology for understanding cellular metabolism and realizing regenerative artificial cells. In this context, our objective was to synthesize

proteorhodopsin (PR), an energy-harvesting protein, through cell-free expression to create an artificial cell capable of generating its own energy within the liposomal space. We confirmed that our system successfully synthesized the PR protein within a single liposome and induced its translocation to the phospholipid membrane, demonstrating the viability of this approach. This study will further present the function and properties of the synthesized PR, elucidate the mechanism of cell membrane translocation, and provide optimization results. The cell-free protein expression model in a single liposome has the potential to evolve into an artificial eukaryotic cell-like model with comparable biological properties, including transcription and translation, as well as metabolic functions similar to natural cells.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **LIFE.P-129**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Bacterial expression of TEV cleavable fluorescent protein pairs for in vitro FRET efficiency study

Yu jeong Kim, Jae-Won Soh*

Department of Chemistry, Inha University, Korea

Fluorescence (Förster) Resonance Energy Transfer (FRET) is a mechanism by which energy is transferred non-radiatively from an excited donor molecule to an acceptor molecule. FRET is dependent on the distance between the donor and acceptor, and can be used to study molecular interactions and distances in the range of 1 to 10 nanometers. We generated bacterial expression vectors for various fluorescent protein pairs and individual fluorescent proteins to study the biochemistry of FRET efficiency between two fluorescent proteins. A bacterial expression vector for the EBFP-mScarlet fusion protein was generated with a linker sequence between the two fluorescent proteins. The linker sequence includes 12 amino acids for flexibility and the ENLYFQG sequence for TEV protease digestion. Expression of the EBFP-mScarlet fusion protein in an E. coli strain, BL21(DE3) was observed by SDS-PAGE. The optimal ratio between the fusion protein and TEV protease was determined for further FRET study. Various spectroscopic parameters such as absorbance and fluorescence were monitored using a UV/VIS spectrophotometer, spectrofluorometer, fluorescence microplate reader, and UV transilluminator. FRET was observed with the crude extract of the EBFP-mScarlet fusion protein. The addition of TEV protease eliminated FRET signals. The cleavage of the EBFP-mScarlet fusion protein into two individual fluorescent proteins (EBFP and mScarlet) was observed by SDS-PAGE. These results suggest that FRET efficiency between two proteins can be studied in vitro using crude extracts and purified proteins.

Poster Presentation : **LIFE.P-130**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Improvement of membrane integrity against physical disruption by ATP-activated actin in artificial cells

Huong Thanh Nguyen, Sang Ho Lee[1], Chang Ho Kim[2], Kwanwoo Shin[1,*]

Chemistry, Sogang University, Vietnam

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

[2]*Institute of Biological Interfaces, Sogang University, Korea*

There is no doubt that the viability of cellular life depends on the preservation of plasma membrane integrity. However, the disruption of the plasma membrane caused by external mechanical or biochemical stressors, and even physiological conditions like cell movement, are always exist which poses an imminent threat to cell survival. Due to its simplicity compared to a living cell, the membrane of artificial cell is more susceptible to damage. Artificial cell membrane can be considerably affected by various factors including surface attachment, electric pulse, chemicals, or membrane proteins which are ubiquitous during the experiments. Under stronger stressors like adsorbing to numerous solid surfaces for example, membrane rupture occurs spontaneously. While living cells possess numerous mechanisms to repair and restore a membrane breach, artificial cells completely lack the machinery to mend the membrane in situations where the pores cannot reseal themselves. In this study, we use ATP-activated globular actin encapsulated inside as a mechanism for instant membrane preservation. Divalent cations were removed from the inner compartment but maintained high concentration outside. Membrane imperfections create pathways for the influx of divalent cations through the breach. This influx will induce the pre-activated G-actin polymerization to form a stable F-actin meshwork that helps maintain pore edge from expanding and prevents the GUV membrane from rupturing. Although the membrane permeability is not totally conserved with actin meshwork, the findings shed light on single cell wound healing mechanisms on artificial cell.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **LIFE.P-131**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Study of Imidazole Salt Characteristics as Pore-Forming Agents for Selective Pore Formation in Liposome

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

The study of pore formation toward bilayer phospholipid can advance the further application of artificial cells in a variety of fields, including cell apoptosis, ion transport, and cell signaling. This work explores the complex selectivity and specificity reactions of four different imidazole salt compositions to three different kinds of vesicles: negatively charged, positively charged, and neutral. We examine the exact distribution of imidazole salt over selected membranes, building on its well-known ability toward membrane permeability. It is especially important because poor specificity is a common problem in most permeability components that target vehicles. We also provide the foundation for the improvement of targeted membrane manipulation by elucidating the subtleties of imidazole salt's specificity. The potential options for breakthroughs in multiple fields of research by revealing the complexities of imidazole salt's selectivity, which in turn sets the conditions for the refining of specific membrane manipulation strategies.

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Poster Presentation : **LIFE.P-132**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Investigation of proteome-tetrazine reactivity for a minimal background biorthogonal click reagent in live cell.

Junyoung Park, Eunha Kim[1,*], Jongmin Park[*]

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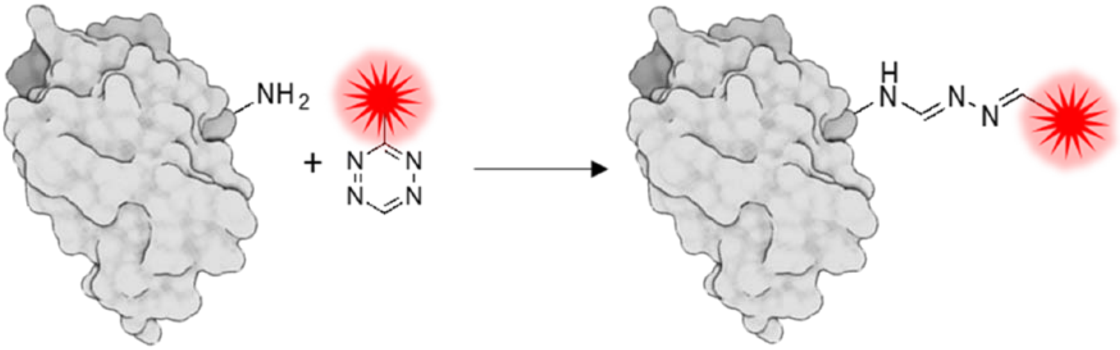
[1]*Department of Molecular Science and Technology, Ajou University, Korea*

Tetrazine undergoes Inverse Electron-demand Diels-Alder (IEDDA) reactions with dienophiles, including trans-cyclooctene (TCO). The IEDDA reaction is one of the click reactions known as bioorthogonal and is being used in various ways, such as observing specific proteins in biological systems or using this reaction as a prodrug strategy. Tetrazine is known to be bioorthogonal. However, some studies have reported that tetrazine is unstable depending on the functional group in the biological environment and Setiz group reported that tetrazine with two methyl esters reacts with nucleophiles such as amines. Based on these studies, we hypothesize that, depending on the structure, tetrazines can react with nucleophiles present in biological systems. Various tetrazine derivatives were synthesized to investigate reactivity with nucleophiles in the biological environment. Every tetrazine was conjugated with silicon rhodamine(SiR) as a fluorescent dye. Using them, we investigated the reaction between tetrazine derivatives and proteins in live cells or cell lysates. In addition, the effect of tetrazine and protein reactivity on protein fluorescence imaging was investigated through an experiment in which BTK protein was labeled.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Poster Presentation : **LIFE.P-133**

Life Chemistry

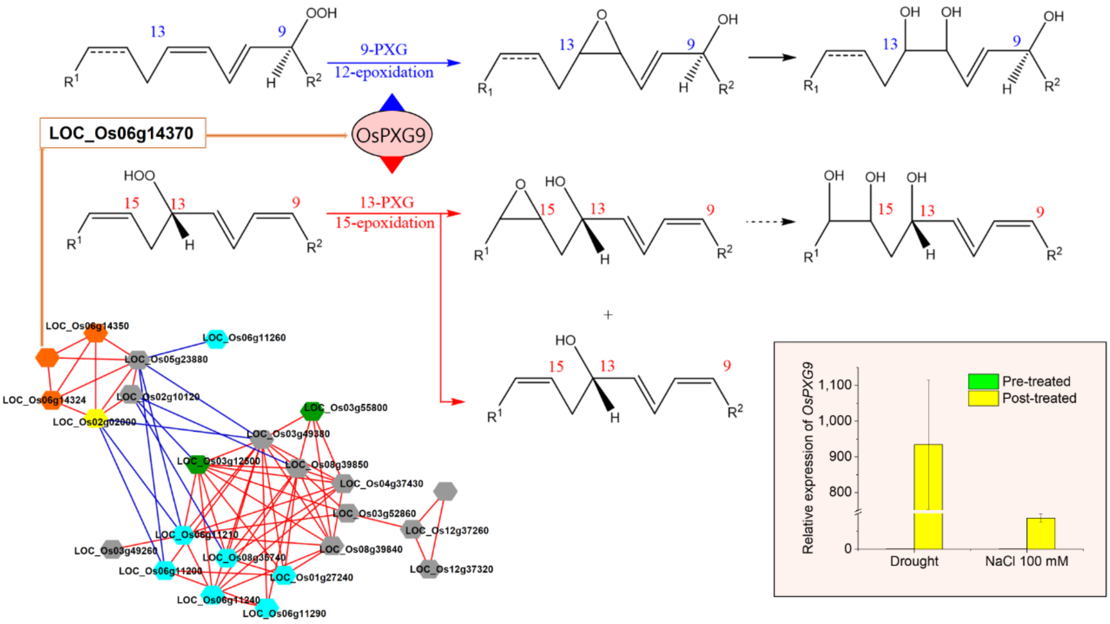
Exhibition Hall 2 FRI 11:00~13:00

Rice peroxygenase catalyzes lipoxygenase-dependent regiospecific epoxidation of lipid peroxides in the response to abiotic stressors

Anh Duc Tran, Oksoo Han*

Department of Molecular Biotechnology, Chonnam National University, Korea

The peroxygenase pathway plays pivotal roles in plant responses to oxidative stress and other environmental stressors. Analysis of a network of co-expressed stress-regulated rice genes demonstrated that expression of OsPXG9 is negatively correlated with expression of genes involved in jasmonic acid biosynthesis. DNA sequence analysis and structure/function studies reveal that OsPXG9 is a caleosin-like peroxygenase with amphipathic α-helices that localizes to lipid droplets in rice cells. Enzymatic studies demonstrate that 12-epoxidation is slightly more favorable with 9(S)-hydroperoxyoctadecatrienoic acid than with 9(S)-hydroperoxyoctadecadienoic acid as substrate. The products of 12-epoxidation are labile, and the epoxide ring is hydrolytically cleaved into corresponding trihydroxy compounds. On the other hand, OsPXG9 catalyzed 15-epoxidation of 13(S)-hydroperoxyoctadecatrienoic acid generates a relatively stable epoxide product. Therefore, the regiospecific 12- or 15-epoxidation catalyzed by OsPXG9 strongly depends on activation of the 9- or 13- peroxygenase reaction pathways, with their respective preferred substrates. The relative abundance of products in the 9-PXG and 13-PXG pathways suggest that the 12-epoxidation involves intramolecular oxygen transfer while the 15-epoxidation can proceed via intramolecular or intermolecular oxygen transfer. Expression of OsPXG9 is up-regulated by abiotic stimuli such as drought and salt stress, but it is down-regulated by biotic stimuli such as flagellin 22 and salicylic acid. The results suggest that the primary function of OsPXG9 is to modulate the level of lipid peroxides to facilitate effective defense responses to abiotic and biotic stressors.


OOH
13
9
R1
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9-PXG
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LOC_Os06g14370
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15-epoxidation
HO
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LOC_Os08g38740
LOC_Os08g39840
LOC_Os06g11200
LOC_Os01g27240
LOC_Os12g37320
LOC_Os06g11240
LOC_Os06g11290
Relative expression of OsPXG9
1,100
1,000
900
800
0
Pre-treated
Post-treated
Drought
NaCl 100 mM

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Poster Presentation : **LIFE.P-134**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Regulation of Microtubules Architecture and Microtubules Bundle Patterns

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

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Microtubule is biopolymer that comprise the cytoskeleton of eukaryotic cells. The cytoskeleton plays a critical role in different types of cells and cellular shape and motility through their dynamic interaction and architecture of actin filament, microtubule and intermediate filament. It is also still unclear how architectures and morphologies of actin networks and microtubules bundles are influenced by spatial confinement and crowded components. In the results from actual cells, actin bundle fibers, stress fibers, can be easily seen, but elongated microtubules bundle fibers cannot be easily observed and are only observed at the edge of the cell. Research results from other groups have shown that microtubule bundles are generated and teardrop patterns are generated through hydrodynamic-flow-inducement. Specially in nerve cells (neuron), long microtubule bundles fibers can be observed in the axons. However, generating and maintaining such significantly long microtubules is not easy. But, our studies of microtubule bundle generation have observed fairly long microtubule bundles and special microtubules bundle patterns in vitro. We think why were able to easily make elongated MTs bundles fibers. One of the factors is hydrodynamic-flow-inducement. This induced radial flow, and we were able to observe microtubule bundles as radial patterns on the surface of the top glass. However, under the Fluronic (F127) coated glass, which prevents MT formation on the top glass, and the dense condition of 10% glycerol, which prevents flow, significantly long rigid MTs bundles were not observed. Their MTs morphology was curly MTs bundles. Now, we can create and control rigid elongated MTs bundles and curly MTs bundles. Additionally, by using slide-glass as top glass, we are able to easily create various patterned coatings on

glass. We plan to create smart pattern coatings on glass slides and generate predictable shapes for microtubule structures and microtubule bundle patterns. Furthermore, by creating an electrode pattern on a slide glass and creating microtubules bundles and microtubules bundle patterns on it to check the electrical characteristics, we aim to provide small clues about the electrical signaling properties of axons in real neurons.

Poster Presentation : **LIFE.P-135**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

In-cell Click-assembled Targeted Protein Degrader for Efficient Protein Degradation

Jaeseok Lee, Jongmin Park[*]

department of Chemistry, Kangwon National University, Korea

Targeted protein degradation (TPD) is a promising therapeutic strategy for addressing intractable diseases by targeting proteins previously deemed undruggable. Proteolysis-targeting chimeras (PROTACs) are a promising approach, consisting of a ligand for the target protein, a linker, and a ligand that recruits an E3 ubiquitin ligase. However, their high molecular weight often poses challenges in terms of cellular uptake, solubility, and pharmacokinetic properties. Our study aimed to develop a novel class of spatiotemporally controllable, click-reaction-based targeted protein degraders. Our approach involved incorporating a photosensitive group and using various linkers that are amenable to bioorthogonal click reactions. Our study successfully synthesized photo-responsive, click reaction-based targeted protein degraders compatible with seven distinct linkers, effectively mediated the degradation of BRD4, a key protein in cancer biology. Our study expands the toolkit of TPD and opens new avenues for the development of precision therapeutics. Our approach allows for the temporal and spatial control of protein degradation by incorporating photosensitive protecting groups, offering a targeted strategy to modulate protein function in a cell-specific and time-resolved manner.

Poster Presentation : **LIFE.P-136**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

tELISA based extracellular vesicle analysis for Renal Cell Carcinoma diagnosis

Soyeon Lee, Jongmin Park*

Department of Chemistry, Institute for Molecular Science and Fusion Technology, Multidimensional Genomics Research Center, Kangwon National University, Korea

Renal Cell Carcinoma (RCC) represents the most prevalent form of kidney cancer, necessitating reliable diagnostic methods for effective management and follow-up postoperatively. Despite the invasive nature and associated risks of complications and costs, biopsy remains the clinical standard for RCC diagnosis. Extracellular vesicles (EVs) present an intriguing avenue for liquid biopsy-based diagnostic biomarker analysis, given their ubiquitous release by various cell types and containing a diverse array of bioactive molecules. However, the identification and characterization of biomarkers for RCC diagnosis utilizing urine-derived EVs remain incompletely understood. In this study, we sought to develop markers for RCC diagnosis through surface protein analysis of urine-derived EVs. Employing the tyramide signal amplification method in conjunction with Enzyme-Linked Immunosorbent Assay (ELISA), a gold standard for conventional EV analysis, we aimed to enhance the sensitivity of marker signal detection, particularly for markers with low expression levels. Utilizing five biomarkers, namely CRP, MCP-1, YKL-40, NGAL, and AQP-1, we conducted an analysis to differentiate RCC patients from non-RCC controls. Furthermore, we also investigated the correlation between these biomarkers and postoperative prognosis, specifically using marker expression at 3 months postoperatively. Our findings demonstrate the efficacy of combining of these five biomarkers present in EVs derived from urine for distinguishing RCC patients from non-RCC controls. Moreover, these biomarkers exhibited promising potential in correlating with postoperative prognosis, thereby offering valuable insights into improving cancer detection and facilitating the postoperative management and follow-up of RCC patients.

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Poster Presentation : **LIFE.P-137**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Challenges in counting of target cell-derived exosome: A protocol for minimized the influence of exosome derived from fetal bovine serum

Ki-ppeum Lee, Jusung An, Hyeonji Rha, Jaewon Kim, Eunji Kim, Changyu Yoon, Yujin Kim, Jiyoung Yoo, Huiyeon Moon, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Exosomes are nano-sized (30–150 nm) membrane vesicles secreted by various types of cells and are thought to play an important role in cell-to-cell communication. Since exosomes reflect the characteristics of the blast cell of origin, tumor-derived exosomes contain various biomarkers such as nucleic acids and proteins that characterize the tumor, and diagnosis using exosomes has been extensively studied. The issue to consider in exosome research is that the amount of exosomes secreted is not fixed, so counting and normalization are essential for accurate analysis. However, there are some challenges in counting or analyzing cell-derived exosomes. The reason is that FBS (Fetal Bovine Serum) used for cell growth has a significant effect on exosome analysis. Even if the exosome-depleted serum is used, FBS-derived exosomes are not completely removed, and a large number (x10^7) of bovine-derived exosomes are present in the isolated exosomes. This causes errors in biomarker analysis. Although many studies overlook this issue, only cell-derived exosomes need to be differentiated for accurate analysis. Therefore, here we propose a protocol to minimize the influence of exosomes derived from FBS for accurate exosome analysis from target cells.

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Poster Presentation : **LIFE.P-138**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Novel Glioblastoma photodynamic therapy agent using non-pi-bond conjugated polymerization

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[1]*College of Medicine, Kyung Hee University, Korea*

Glioblastoma (GBM) stands as a highly lethal grade 4 tumor, posing significant challenges to treatment with its rapid progression and poor survival rates. Current therapeutic avenues for GBM encompass surgical resection, radiation therapy, chemotherapy, and emerging techniques like photodynamic therapy (PDT). Especially, PDT, which induces cell death by generating reactive oxygen species (ROS) by utilizing photosensitizers (PS) activated by specific light wavelengths, is emerging as a promising method to remove remaining tumor cells more safely after surgery. To optimize the efficacy of effective PS molecules utilized in PDT, it is important to minimize the energy gap between singlet and triplet excited states to increase the efficacy of the intercrossing system, which can lead to higher PDT efficacy.In this study, polymeric amino-single-benzene nano-aggregates (PANA) as a novel PS backbone for glioblastoma PDT was developed. As a method to increase the efficacy of PS, a repeating bond of a single benzene was formed during the non-pi-bond conjugated polymerization reaction, and the blood-brain barrier (BBB) penetration efficiency was improved through LAT 1 (Large Amino Acid Transporter 1) by including many amine groups.PANA was synthesized by a facile one-pot reaction and produces nano aggregates with high stability and glioblastoma specificity. Through in vitro analysis, the strong efficacy of PANA as PS, which induces ROS generation upon laser irradiation, was proven, and this was also confirmed by theoretical calculation results to show that the ISC rate constant increases significantly as polymerization of PANA progresses. Based on this, in vivo experiments showed that the high PDT efficacy of PANA induced GBM cell death and extended the lifespan of GBM xenografted mice. These findings suggest PANA as a promising PDT PS and reveal a new strategy for developing new PSs.Ref: Bioactive Materials, 2023, 24, 497-506

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Poster Presentation : **LIFE.P-139**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Engineering Cellular Microenvironment and Intercellular Interactions through $\alpha_5\beta_1$ Integrin Overexpression in Human Dermal Fibroblast

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Department of Chemistry & Institute of Biological Interfaces, Sogang University, Korea

In the field of 3D cell and organoid assembly, the interaction between cells and their microenvironment, such as the extracellular matrix (ECM), is a crucial factor in the successful self-organized growth of cell in vitro. Recent studies have demonstrated that the pivotal role of $\alpha_5\beta_1$ integrin and soluble fibronectins in cell-ECM force generation and ECM polymerization. To enhance cell-ECM interaction, we overexpressed $\alpha_5\beta_1$ integrin in human dermal fibroblast (HDF) cells using recombinant lentiviruses. The resulting α_5 and β_1 overexpressed cells were selected using G418 selection method to establish a stable cell line, which was then analyzed for α_5 and β_1 expression using western blotting. The results showed that overexpression of integrin altered the phenotype of the HDF cells, including size and proliferation rate, and resulted in an increase in ECM proteins such as fibronectin and collagen. The enhance interaction between cells and their environment observed in the integrin overexpressed cells can be utilized to construct ECM-rich 3D cell assemblies.

Poster Presentation : **LIFE.P-140**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Pentafluoro-benzene Functionalized AIEgen as a Rapid and Highly Sensitive Fluorescent Nanoprobe for Gold Ion Detection

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Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Gold-related chemical research has grown in the past decade, particularly for medical applications. While gold ions have anti-inflammatory properties, their ionic forms (Au(I) and Au(III)) can be reactive and pose health risks. Despite existing detection methods, developing new fluorescent probes for efficient and sensitive detection of gold ions remains challenging. In this research, we presented a novel fluorescent nanoprobe (named AuP-2) designed for the detection of gold ions (Au(III)). Utilizing a pentafluoro-benzene functionalized AIEgen (aggregation-induced emission luminogen), the nanoprobe exhibited notable attributes such as high selectivity, sensitivity (5.924 ppb), and a rapid response time (within 10 seconds). The interaction between alkynophilic Au(III) and the electron-deficient pentafluoro-benzene moiety played a pivotal role in disrupting the AIEgen stacking and inducing a turn-off emission response. AuP-2 demonstrated exceptional biocompatibility with low toxicity towards COV-318 (ovarian cancer cells) and showcased its capability to visualize the Au-complex drug (auranofin) within cells. Practical applications extended to superior sensing of Au(III) in diverse natural water samples, paper-based strips, and natural soil samples. In conclusion, AuP-2 could emerge as a promising sensor for Au(III) detection in both fundamental research and industrial contexts, underscoring its versatility and suitability for Au(III)-related chemical and industrial investigations. Ref: Dyes and Pigments, 2022, 198, 110007

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Poster Presentation : **LIFE.P-141**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Construction of ASBBFs (Amino-Single Benzene-based Fluorophore) Library

Jaehui Lee, Dokyoung Kim[1,*]

Precision Medicine, Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Single benzene-based fluorophores (SBBFs) have garnered attention recently for their unique photophysical properties. These properties include exceptional photostability, resilience to environmental influences, and high quantum efficiency. However, conventional organic fluorophores often face limitations in biological applications due to increased hydrophobicity. In this study, we introduce a novel library of amino-substituted SBBFs (ASBBFs) with an electron donor-acceptor structure within a single benzene ring. We investigated the synthesis methodology, analyzed its photophysical characteristics, performed quantum chemical analyses, and evaluated its compatibility for two-photon excitation and cellular imaging applications. We anticipate the versatility of ASBBFs as fluorophores across various fields, providing essential guidelines for future advancements and utilization in fluorophore research.

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Poster Presentation : **LIFE.P-142**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Iron-Silicate Coated Porous Silicon Nanoparticles: A Novel Approach for Enhanced In Situ ROS Generation and Anticancer Efficacy

Jihyun Lee, Eun-Kyoung Bang[1,*], Dokyoung Kim[2,*]

KHU-KIST Department of Converging Science and Technology, Graduate School, Kyung Hee University, Korea

[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

[2]*College of Medicine, Kyung Hee University, Korea*

We introduce iron-silicate-coated porous silicon nanoparticles (Fe-pSiNPs-NCS) as a pioneering approach for enhanced reactive oxygen species (ROS) generation within cancer cells, leveraging the Fenton-like reaction capabilities of iron-silicate. This advancement is achieved through the surface modification with iron-silicate and 3-isothiocyanatopropyltriethoxysilane (TEPITC), significantly amplifying ROS production via a catalytic Fenton-like reaction. The process not only elevates H2O2 levels but also strategically decreases intracellular glutathione (GSH) levels, which are known to reduce ROS, thereby intensifying oxidative stress selectively in tumor cells. Our investigation reveals Fe-pSiNPs-NCS's potent cytotoxic impact on U87MG cancer cell lines due to this enhanced ROS self-generation mechanism. Furthermore, we validate the utility of Fe-pSiNPs-NCS as a versatile drug delivery platform, exhibiting high loading efficiency for chemotherapeutic agents like doxorubicin and SN-38. These findings underscore the Fe-pSiNPs-NCS as a versatile platform for both targeted cancer therapy and as a carrier in drug delivery systems. Our work paves the way for innovative nanotherapeutic strategies in the biomedical field, offering a new paradigm in the design of ROS-generating nanomaterials for cancer treatment. References: Um, H. et al., Colloid Surf. B-Biointerfaces, 2023, 225, 113273.

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Poster Presentation : **LIFE.P-143**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Innovative urine-based femetch: a novel nitrobenzene-based fluorescent biothiol probe with controlled Smiles Rearrangement

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Precision medicine, Kyung Hee University, Korea

[1]*College of Medicine, Kyung Hee University, Korea*

Femetch (female technology) is an industry or field that provides technological solutions to improve women's health and well-being. We developed the novel fluorescent diagnostic probe, NPS-B, tailored for urine-based cervical cancer diagnosis. This nitrobenzene-based probe responds differentially to cysteine (Cys) and homocysteine (Hys) in human urine through controlled Smiles Rearrangement. While these biomarkers, biothiols, are present in urine mixtures, the shorter distance between the amino and thiol groups in Cys (4.17 Å) compared to Hys (5.25 Å) results in a faster SR reaction. However, the rapid reaction kinetics pose challenges as both the N-adduct product and S-adduct intermediate form emit light at similar wavelengths, confounding differentiation efforts. To address this, pivotal modifications were made to two constituent elements of 4-chloro-7-nitrobenzofurazan. Aromatic substitutions with electron-donating group (EDG) characteristics were introduced to the para position of the NO2 in nitrobenzene, altering the electron density and inducing nucleophilic aromatic substitution (SnAr) reactions. Additionally, by substituting the O atom of the nitrobenzene backbone with a Se atom, which possesses greater polarity, we achieved a slow and delayed internal charge transfer (ICT) effect. As a result, when NPS-B reacts with Cys and Hys, a transition state was maintained via the controlled SR reaction, allowing emission at different wavelengths (560nm and 630nm, respectively) for the N- and S-adducts.

Poster Presentation : **LIFE.P-144**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of Turn-On Fluorescent Nanoprobe AgP-1 for Selective Silver Ion Detection

Yeonjin Lim, Dokyoung Kim[1,*]

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[1]*College of Medicine, Kyung Hee University, Korea*

Humans have utilized silver for millennia in various industries due to its unique properties, notably in pharmaceuticals for its antibacterial, antiviral, and antifungal properties. However, uncontrolled exposure to silver ions (Ag+) can lead to adverse health effects, necessitating the development of selective detection methods. This study introduces AgP-1, a novel fluorescent nanoprobe capable of selectively detecting silver ions in biological media. This innovative probe, composed of AIEgen (tetraphenylethylene; TPE) and 2-(methylthio)aniline (MTA), efficiently detects silver ions through secondary amine formation. Utilizing a hybrid structure, AgP-1 demonstrates a significant fluorescence enhancement upon Ag+ binding, due to restricted rotation and enhanced stacking of the TPE core. AgP-1 forms aggregates in a fluorescence off-state in an aqueous solution, but AgP-1 exhibited enhanced fluorescence when binding with silver ions in biological environments. This probe exhibits excellent performance characteristics, including a low detection limit (6.6 ppb), rapid response time (within 10 seconds). Moreover, it exhibited low toxicity towards glioblastoma cells and efficiently visualized silver ions in cancer cells (U87MG) and bacteria (S. aureus). AgP-1 offers high selectivity, sensitivity, rapid response time, biocompatibility, and applicability in bio-imaging. This nanoprobe emerges as a promising tool for silver-related research in both chemical and biological domains, offering significant potential for various applications in bio-imaging. References.Kim, Na Hee. et al., Dyes and Pigments., 2022, 2, 110027.

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Poster Presentation : **LIFE.P-145**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Self-Activating Therapeutic Nanoparticles (SATNs): Advancing ROS-Mediated Nanomedicine for Enhanced Tumor Therapy

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[1]*College of Medicine, Kyung Hee University, Korea*

Over the past few decades, scientists have devoted significant attention to nanotherapeutics and nano-based drug delivery platforms, leading to advancements in controlled drug release and targeted delivery of bioactive substances. Reactive oxygen species (ROS) have emerged as crucial regulators of cellular functions, impacting signal regulation, cell proliferation, and survival. Elevated ROS levels can disrupt cellular homeostasis and induce cell death, making them valuable in disease-related research, particularly in nanotherapeutics. In chemotherapy, ROS act as potent endogenous anti-cancer agents by inhibiting tumor growth and inducing cell death. Various strategies aim to elevate endogenous ROS levels in anticancer therapies, including light-induced singlet oxygen generation and hydroxyl radical generation. However, due to limitations, there's a need for new nanoformulations capable of generating ROS without external initiators, efficiently targeting cancer cells, and being biodegradable.This study introduces self-activating therapeutic nanoparticles (SATNs), demonstrating effective cancer celltargeting, endogenous ROS generation, and ROS-induced drug release. SATNs are systematically functionalized with ROS-reactive nanocarriers, utilizing porous silicon nanoparticles (pSiNPs) that undergo biodegradation. Loaded with ROS-responsive prodrugs, SATNs exhibit anti-cancer effects in pancreatic cells, with tumor site accumulation and therapeutic efficacy without histological toxicity or hepatotoxicity. This study presents a novel strategy for ROS-mediated nanomedicine, offering a promising approach for tumor therapy with enhanced targeting and therapeutic efficiency.

Poster Presentation : **LIFE.P-146**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

High resolution mapping of α-synuclein phosphorylation using single-molecule fluorescence

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α-synuclein is a protein mainly found in the brain. It plays a crucial role in neurodegenerative diseases like Parkinson's. It is known to form abnormal aggregates within neurons, disrupting cellular processes, and impairing synaptic function. The physiological function of α-synuclein is modulated by phosphorylation, which alters its structure, interactions, and cellular roles. Studying the effects of phosphorylation on the structure and function of α-synuclein will deepen our understanding of its biological roles and its dysregulation in disease states. The function of α-synuclein is dependent on the position and number of phosphorylation sites; however, analyzing the profile of multi-phosphorylation remains challenging, necessitating high-sensitivity techniques.Single-molecule biophysics offers exceptional sensitivity in the analysis of individual protein molecules, revealing hidden dynamics and interactions inaccessible to traditional biochemical measurements. We utilize single-molecule FRET (Förster resonance energy transfer) techniques to determine distances between detection spots and create fingerprinting maps to assess the number of sites of interest. We combine this technique with site-specific labeling of phosphorylation, enabling high-resolution mapping of α-synuclein phosphorylation at the single-molecule level.

Poster Presentation : **LIFE.P-147**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Building Proteins with Native Chemical Ligation *in vitro*

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Protein synthesis has gained interest over the last two decades due to its ability to yield high-value bioproducts. This effort has been pursued through two primary chemical methods: i) the chemical synthesis of peptide fragments, and ii) the utilization of native chemical ligation to fuse two peptide fragments into a larger structure. However, producing these peptide fragments using solid-phase platform is inefficient, thus, the range of proteins obtained through this strategy has remained limited. Herein, we introduce a new biochemical technique that combines native chemical ligation with a cell-free protein synthesis (CFPS) platform. We employ the genetic code reprogramming approach on a cell-free platform where release factor 1 is absent to produce peptide fragments that fuse together with a covalent amide bond. This results in a peptide:tRNA complex bearing a reactive C-terminal ester. We have recently discovered that these peptide:tRNA complexes react with Cys, forming an amide bond and successfully releasing the tRNA from the complex. We believe this work will provide an efficient way to synthesize high-value products such as proteins containing multiple D-amino acids.

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Poster Presentation : **LIFE.P-148**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

High yield purification of poly(ethylene) terephthalate hydrolase from the periplasm of *Escherichia coli*

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The exponential increase in plastic waste has led to environmental and ecological problems. Enzymatic degradation of plastic waste provides a sustainable solution for poly(ethylene) terephthalate (PET) waste recycling. Nevertheless, the application of PET hydrolase (PETase) has been hindered by its low yield and stability. Here, we report the production of maltose binding protein (MBP) fusion PETase, either with or without the N-terminal signal peptide in the periplasm or cytoplasm of Escherichia coli. The MBP fusion PETase exhibited a higher expression level at 289 K compared to the wild type PETase with a hexahistidine tag. Additionally, we demonstrated that MBP fusion PETase with the N-terminal signal peptide can be purified from osmotic shock fluid by immobilized metal affinity chromatography to a high purity level. Furthermore, we determined kinetic parameters using the Michaelis-Menten equation as follows: V_{max} = 47.2 μM min^{-1}; k_{cat} = 78.7 s^{-1}; K_m = 3.0 mM. The catalytic efficiency of MBP fusion PETase is 1.8 times higher than the wile type enzyme. Our works will be applied to develop an E. coli strain for degrading PET.

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Poster Presentation : **LIFE.P-149**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Light-Triggered RNS/ROS Release and Simultaneous Intramitochondrial Self-Assembly of Nanostructures for Supramolecular Cancer Therapeutics

Dohyun Kim, Ja-Hyoung Ryu[1,*]

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Utilizing gaseous signaling molecules (GSMs) for gas therapy and achieving organelle-targeted self-assembly of nanosized objects as "unconventional" therapeutics through light-induced spatiotemporal control holds the potential to introduce novel and innovative therapeutic approaches. Yet, the unexplored territory lies in combining gas therapy and concurrent assembly of nanosized objects within the intricate cellular microenvironment, entwined with cellular functions and their interplay with cellular components, all in pursuit of therapeutic goals. Here we present, the light triggered delivery of RNS (i.e., NO) and ROS (i.e., 1O2) followed by organelle-localized self-assembly of small amphiphiles as a strategy for control-ling cellular fate. We synthesized visible light induced on-demand NO-releasing amphiphiles, termed as Mito-C6-NO & Mito-C18-NO. Notably, Mito-C18-NO emerges as a robust candidate, exhibiting heightened cytotoxicity and inducing mi-tochondrial dysfunction via membrane disruption to drive apoptosis, which could be attributed due to the synergistic interplay of NO and 1O2 release, culminating in the spontaneous generation of nanostructures from Mito-C18-H. Our or-ganelle-specific supramolecular system introduces a promising avenue for therapeutic interventions and in-depth exploration of cellular mechanisms. Light induced NO-release mechanism as well as formation of nano structures have been investigated by density functional theory and molecular dynamics simulations.

Poster Presentation : **LIFE.P-150**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Exploring Liquid-Liquid Phase Separation in Organic Solvent Environments

Soobeen Lee

Kyung Hee University, Korea

Liquid-liquid phase separation (LLPS) is a complex phenomenon intertwined with various cellular processes, garnering attention for its potential applications in drug development and disease research. However, the predominant focus on aqueous environments limits its utility. Recent efforts that expands LLPS research into organic solvents would reveal insights into how solvent polarity influences LLPS mechanisms. This exploration opens avenues for LLPS utilization in organic synthesis, biological reactions, and potentially chirality control, demonstrating its broad applicability beyond aqueous systems.

Poster Presentation : **LIFE.P-151**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

An Efficient Lysate-Based Cell-Free Synthesis Platform for Site-Specific Incorporation of Unnatural Substrates into Proteins

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

Cell-free protein synthesis (CFPS) system enables the site-specific incorporation of unnatural substrates into a peptide or protein. Site-specific incorporation of an artificial substrate using synthetic tRNAs on a lysate-based cell-free platform is inefficient because synthetic tRNAs compete with endogenous tRNAs. A commonly used method to avoid such competition is to use a reconstituted cell-free system (e.g., PURExpress) in which natural amino acids (aa) are selectively excluded, thereby preventing them from forming an endogenous tRNA:aa complex. However, producing peptides or proteins bearing unnatural substrates using the PURE system is costly and inefficient (i.e., low protein yields). Herein, we demonstrated an efficient and inexpensive lysate-based cellfree synthesis platform in which the competition between endogenous and synthetic tRNA is eliminated. Specifically, we aim to insert a purification tag into the gene of aaRSs in the Escherichia coli genome and remove them selectively so that no endogenous aaRS:aa complex is further produced in the cell lysate. This new platform will enable the efficient synthesis of a wide variety of novel bio-based materials bearing synthetic substrates.

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Poster Presentation : **LIFE.P-152**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Creating a novel fluorescent probe capable of instantly detecting both O-GlcNAcase and phosphatase activities.

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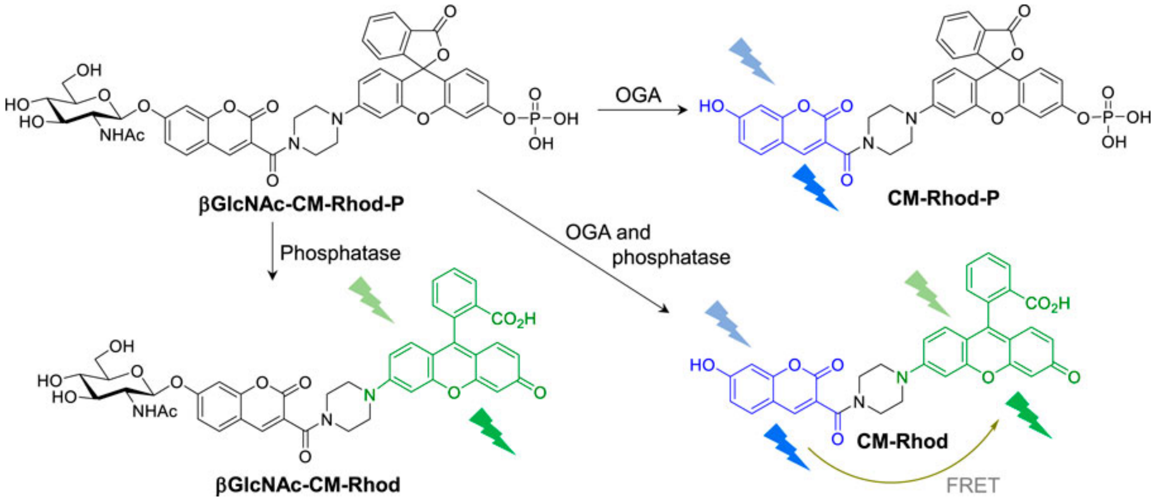
The modification of proteins by O-GlcNAc often intersects with protein phosphorylation, both of which are dynamic posttranslational events regulating various cellular processes. Given the physiological and pathological importance of protein O-GlcNAcylation and phosphorylation, we developed the fluorescent probe βGlcNAc-CM-Rhod-P to selectively detect the activities of O-GlcNAcase (OGA) and phosphatase, the enzymes responsible for these modifications. βGlcNAc-CM-Rhod-P consists of a βGlcNAc-conjugated coumarin (βGlcNAc-CM) as an OGA substrate, a phosphorylated rhodol (Rhod-P) as a phosphatase substrate, and a piperazine bridge. The distinct emission wavelengths of CM and Rhod liberated from the probe (100 nm difference) prevent spectral interference. Our study revealed that treatment of βGlcNAc-CM-Rhod-P with OGA leads to the formation of the GlcNAc-cleaved probe, CM-Rhod-P, accompanied by an increase in fluorescence intensity from free CM. Similarly, exposure to phosphatase results in a dephosphorylated probe, βGlcNAc-CM-Rhod, with strong fluorescence from free Rhod. When incubated with both enzymes, βGlcNAc-CM-Rhod-P is converted to CM-Rhod, lacking both βGlcNAc and phosphoryl groups, with increased fluorescence from both free CM and Rhod. This probe effectively detects OGA and phosphatase activities in cell lysates and enables fluorescent imaging of both enzymes in cells. Overall, βGlcNAc-CM-Rhod-P serves as a valuable chemical tool for simultaneous assessment of OGA and phosphatase activities.


βGlcNAc-CM-Rhod-P
OGA
CM-Rhod-P
Phosphatase
OGA and phosphatase
βGlcNAc-CM-Rhod
CM-Rhod
FRET

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Poster Presentation : **LIFE.P-153**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Study of the senescence progress of human skin fibroblast on silica nanobeads array

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Senescence is a physiological process that progresses with age. Cellular senescence is induced by stimuli such as telomere shortening and oxidative stress. In particular, it refers to the cell cycle arrest state. Senescence cells are characterized by reduced cell proliferation, migration, and speed. In addition, aging proteins p16, p21, and p53 are expressed.We study the adhesion changes of senescence cells on silica nanobeads (SiNBs) of various sizes. In particular, it analyzes how senescence changes due to different adhesion. We induced aging by adding Paclitaxel (PTX) to WS1 cells, which are human skin fibroblasts. PTX causes cellular senescence due to damage from ROS. The optimal PTX concentration was fixed, and the cell survival rate was confirmed by MTT assay. In particular, we have identified different adhesion on SiNB arrays of various sizes. In addition, changes in cell proliferation, migration, speed, and aging proteins were analyzed. As a result, we observed the correlation between the topographic factors of SiNB arrays and cellular senescence.

Poster Presentation : **LIFE.P-154**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Simulation and Application of Red Fluorescent Nanodiamonds for Temperature Sensing in Skin Cells via Microwave-Assisted Techniques

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Fluorescent nanodiamonds(FNDs) have emerged as promising candidates for various biomedical applications owing to their exceptional stability and advantageous properties. In this study, involves the incorporation of FNDs into skin cells and utilizing them as probes for temperature changes. The cells are seeded on Coplanar Waveguide (CPW) substrate and subjected to microwave irradiation. Through this setup, we aim to modulate cellular behavior or measure characteristic changes by monitoring alterations in magnetic fields induced by the interaction between the cells and the FNDs. To expedite the experimental design and optimization, simulations using the COMSOL Multiphysics software are conducted, providing insights into the dynamics of the proposed setup. The utilization of FNDs in cellular sensing offers several advantages. Non-invasive internalization into cell, the robustness and biocompatibility, and the unique optical properties of FNDs, particularly their stable and bright fluorescence, enable precise detection and imaging within cellular systems. Beyond temperature sensing, FNDs can be tailored for detecting various biomolecules, monitoring cellular dynamics, and even delivering therapeutic agents with unprecedented precision.

Poster Presentation : **LIFE.P-155**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Intracellular uptake mechanism of an artificial virus model conjugated with a spike protein derived from SARS-CoV-2

Eunjin Kim, Albertus Ivan Brilian, Ignasia Handipta Mahardika, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Coronaviruses have triggered significant health crises, exemplified by the COVID-19 pandemic. Viruses like SARS-CoV-2 possess spike proteins on their outer surface, facilitating infection through selective binding to immune cells and subsequent cellular uptake. However, actual viruses cannot be readily available for demonstrating and studying this infection mechanism. Therefore, creating artificial viruses with similar structures and functional groups becomes an urgent need for laboratory studies. In this presentation, we employed lipid nanoparticles (LNPs) to construct an artificial coronavirus model, resembling the size and biochemical properties of SARS-CoV-2. Protein derivatives extracted from the spike protein of SARS-CoV-2 were conjugated to phospholipids to investigate their interaction with mammalian cells and the intracellular uptake mechanism. Through fluorescent labeling, the intracellular penetration of the LNPs was readily observed using high-resolution STED and confocal microscopy. We found that the presence of conjugated spike proteins induced successful penetration not only through the plasma membrane but also through the intracellular nuclear membrane. The significance of this study lies in its ability to provide a safer and more scientifically rigorous exploration of viral infection mechanisms, with potential applications in the development of new vaccines or targeted gene delivery.Keywords: COVID-19, Virus, LNP, Virus model, Drug delivery system

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Poster Presentation : **LIFE.P-156**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Novel spray coating technique for large-area homogeneous adsorption of fibronectin for enhanced wound healing

Chaeeon Lim, Albertus Ivan Brilian, Sang Ho Lee, Kwanwoo Shin[*]

Department of Chemistry, Sogang University, Korea

The extracellular matrix component fibronectin (FN) plays a pivotal role in the overall wound healing process as an adhesive glycoprotein, essential for the formation of the extracellular matrix and the re-epithelialization of wounds, thereby accelerating the healing rate. Thus, integrating FN into surgical sutures could enhance cellular migration and adhesion at the wound site, promoting accelerated wound recovery. However, the current predominant method of FN-coating, immersion coating, is difficult to produce a homogeneous and even coating on surface and results in significant waste or loss of the coating material. In this study, we aimed to create functional surfaces containing FN for wound healing by applying a spray technique to easily coat large-area surfaces with ECMs such as FN, including surgical sutures and various target substrates. In this experiment, after spraying FN solution on sutures, we visualized the successful deposition of fibronectin on the surface by scanning electron microscopy (SEM) and fluorescence conjugation. Moreover, irradiation of the suture surface with UV/ozone (UVO) created a hydrophilic surface, allowing for a more effective attachment of FN. Based on these results, the spraying technique for FN coating suggests the potential development of functional medical products that could enhance the wound healing outcomes.Keywords: fibronectin, extracellular matrix, spray

Poster Presentation : **LIFE.P-157**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Simulating Subcellular Compartmentalization: Endocytosis Modeling in Fibronectin-Coated Phospholipid Artificial Cells

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Department of Chemistry, Sogang University, Korea

Intracellular compartmentalization, essential for the complex functionality of eukaryotic cells, involves partitioning the cell interior into membrane-enclosed organelles to enhance metabolic efficiency and functional diversity. To achieve artificial cells with intracellular compartmentalization, one potential approach is to induce various forms of pseudo-endosomes inserted from the outer membrane into the interior. Therefore, we utilized the cell membrane of giant unilamellar vesicles (GUVs) made of a single unilamellar phospholipid to induce budding into the cytoplasm, a process analogous to endocytosis, mimicking the morphology and structure of endosomes formed from the outer membrane. Osmotic pressure was applied to shrink the volume of GUV, an artificial cell model, inducing the outer cell membrane to vesiculate inside, as observed under a confocal microscope. To prevent GUVs from rupturing under osmotic pressure, we electrostatically coated the GUVs with fibronectin, an extracellular matrix (ECM), enhancing the flexibility and strength of the membrane. This research not only enhances the feasibility of creating artificial cells closely resembling real cells but also holds implications for biomimetic cells with intracellular compartmentalization.Keywords: intracellular compartmentalization, endocytosis, fibronectin, giant unilamellar vesicle

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Poster Presentation : **LIFE.P-158**
Life Chemistry
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Colorectal cancer-derived extracellular vesicle protein analysis by sandwich type SERS immunoassay

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[1]*Department of Chemistry, Kangwon National University, Korea*
[2]*department of Chemistry, Kangwon National University, Korea*

Extracellular vesicles (EVs) are secreted from cells and are abundant in the blood, containing proteins, nucleic acids, and lipids from the parent cell. Analyzing EVs in the blood can provide information about the disease non-invasively. This makes EVs a promising circulating biomarker. However, there are many other EVs in the blood besides disease-associated EVs, so it is important to sensitively detect disease-associated EVs in the blood. Surface-enhanced Raman scattering (SERS) is a non-destructive, sensitive technique that allows analysis even with small amounts of sample. In addition, it is also multiplexable and has been used a lot in EV analysis recently. In this study, colorectal cancer EV surface protein was detected by sandwich type SERS assay using Au nano wire substrate and SERS tag. As a result, it showed better detection performance compared to ELISA, which is the gold standard for EV analysis. Furthermore, by comparing the expression of marker protein in colorectal cancer cells and the expression of marker protein in colorectal cancer cell EVs, we confirmed that EVs reflect the protein expression of parent cells. Then, we checked the expression of the marker protein using EVs obtained from colorectal cancer patient plasma and normal control plasma, and confirmed that it was possible to distinguish between normal and cancer.

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Poster Presentation : **LIFE.P-159**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

3T3 cellular behavior on the various curvature-modified Liquid Phase Deposition

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

Individual cells and multicellular systems respond to cell-scale curvatures in their environments, guiding migration, orientation, and tissue formation. However, it remains largely unclear how cells collectively explore and pattern different curvatures. Here, we demonstrate the focal adhesion dynamics of fibroblast cells onto nanostructured surfaces of hexagonally close-packed silica bead arrays using a liquid-phase deposition (LPD) method with 3T3/NIH cells. We quantify curvature-induced patterning and find that cells generally prefer regions with at flat curvature. However, we also show that cell migration is faster on convex topography than on flat surfaces. We demonstrate that this is partly regulated by cellular contractility and extracellular matrix development, underscoring the mechanical nature of curvature guidance. Our findings offer a geometric perspective on cell-environment interactions that could be harnessed in tissue engineering and regenerative medicine applications.

Poster Presentation : **LIFE.P-160**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Visualizing large DNA molecules through Scanning Electron Microscopy (SEM) Using a Metal-Free Electro-Stain Composed of DNA-Binding Proteins and Synthetic Polymers

Chanyoung Noh, **Kyubong Jo**[1,*]

Sogang University, Korea

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

DNA visualization is crucial in genomic research. We have developed a novel electro-stain reagent for visualizing DNA using a scanning electron microscope (SEM). This reagent is created by combining DNA-binding proteins with synthetic polymers, which improves the visibility of DNA strands, which are typically 2 nm thick, when viewed under SEM. Unlike conventional staining reagents for electron microscopy that rely on heavy metals, our method utilizes proteins and polymers to stain DNA, resulting in dark lines when viewed under SEM. The resulting images show a thickness ranging from 15.0±4.0 nm. As SEM serves as the primary platform, it seamlessly integrates with various chemically treated surfaces and microfluidic devices. Our technique enables high-resolution imaging of different DNA configurations, including linear, circular, single-stranded, and double-stranded, as well as various DNA structures, ranging from genomic and mitochondrial DNA to chromatin and chromosomes. Additionally, quantum dots were successfully visualized as bright labels specifically incorporated into the polymer-stained DNA molecules. In summary, SEM DNA imaging using this innovative electro-staining technique provides electron microscope resolution with the convenience of optical microscopy.

Poster Presentation : **LIFE.P-161**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Molecular Design Strategy for Iridium(Ⅲ)-based Photosensitizers to Enhance the Phototoxicity Index and Efficacy of Photodynamic Therapy.

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

In photodynamic therapy (PDT), the efficacy of the photosensitizer depends on a phototoxicity index (PI), indicating a gap between the IC50 values of phototoxicity and cytotoxicity in the absence of light, commonly referred to as dark toxicity. Iridium(Ⅲ)-based photosensitizers (PS) hold promise for PDT treatment, with notable efficiency in generating reactive oxygen species (ROS). Nevertheless, certain Ir(Ⅲ)-based photosensitizers have dark toxicity problem. High dark toxicity not only reduces the efficiency of PDT by lowering the PI value but can also increase side effects by affecting off-targets. Thus, there arises a necessity for guidelines to autonomously regulate the dark toxicity of photosensitizers. Herein, we present a novel molecular design strategy aimed at diminishing dark toxicity and amplifying the photo-toxicity of Ir(Ⅲ)-based photosensitizers by modulating their charge and integrating specific organelle-targeting groups. Through alterations in molecular charge, we have discerned that neutrally charged PSs evince markedly reduced dark toxicity relative to positively charged PSs. Furthermore, the incorporation of cell organelle-targeting groups enhances the photo-toxicity of neutrally charged PSs. Consequently, we affirm that optimizing the structure of Ir(Ⅲ)-based photosensitizers for PDT efficacy necessitates meticulous control over these two parameters.

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Poster Presentation : **LIFE.P-162**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Capillary Force Driven Microfluidic Device for Analysis of Large Single-Molecule DNA

Taesoo Kim, Kyubong Jo*

Department of Chemistry, Sogang University, Korea

Rapid advancements in microfluidics are propelled by its extensive applications in life sciences and biomedical engineering. A key challenge within microfluidics is the precise control and manipulation of fluids in microscale channels. Addressing this challenge, capillary force-driven flows offer a promising solution, obviating the need for external power sources. These capillary-driven flows are particularly advantageous for the consistent and reliable analysis of single-molecule DNA when integrated with a fluorescence microscope, offering a straightforward yet potent method. In this study, we have developed multiple microfluidic devices utilizing capillary force to enhance the deposition of DNA molecules onto positively charged glass surfaces from sample solutions. Optimization efforts focused on outlet reservoir capacity, surface charge density, and microchannel dimensions. These refinements enabled us to maximize DNA elongation and deposition, achieving a detection limit of 0.48 fg/μL, equivalent to 64 molecules of 7.25 kbp DNA in 1 μL, distinguishable by DNA length. The developed device serves as an ultra-sensitive platform for quantitative DNA analysis and facilitates rapid, accurate point-of-care testing with minimal detection limits. In summary, our findings underscore the potential of capillary force-driven microfluidics for reproducible and efficient fluid manipulation within microscale channels.

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Poster Presentation : **LIFE.P-163**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Exploring Liquid-Liquid Phase Separation: Innovative Paths for Ring-Opening Polymerization of NCAs

Honggi Jeon

Applied Chemistry, Kyung Hee University, Korea

Proteins containing modular domains or intrinsically disordered regions, along with nucleic acids, play a pivotal role in initiating the formation of membraneless condensates through liquid-liquid phase separation (LLPS). This mechanism is crucial for the assembly of cellular organelles and other condensates, providing insights into the dynamic organization of cellular components. The driving force involves various interactions (pi-pi, hydrophobic, cation-pi, dipole-dipole, etc.), leading to the emergence of distinctive features in the condensates. Due to the high solute concentration, specific environments take shape within the condensates, determined by the characteristics of the involved proteins. We investigated additional environmental distinctions between the condensates and the solvent in LLPS, discovering the potential for applying this to the ring-opening polymerization (ROP) of N-carboxyanhydrides (NCAs). Consequently, we will introduce a novel ROP of NCAs utilizing the LLPS system.

Poster Presentation : **LIFE.P-164**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Divalent Cation Regulation of Actin Filamentary Bundles and Networks

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[1]*Institute of Biological Interfaces, Sogang University, Korea*

Divalent ions, particularly calcium (Ca^{2+}) and magnesium (Mg^{2+}), play a crucial role in the structural and functional dynamics of mammalian cells by regulating actin filament bundles and networks within the cytoplasm. Actin filaments, crucial for cytoskeletal support, external stress resistance, and cell migration, are significantly influenced by the concentration of G-actin and the presence of Mg^{2+}. The macroscopic nature of fiber formation at high concentrations, observed using conventional fluorescence microscopy, has made it challenging to fully comprehend the structure at the molecular scale and the mechanism of fibril formation at early stage. In this study, we employed advanced imaging techniques such as TEM, confocal, and STED microscopy to investigate the impact of variations in G-actin and Mg^{2+} concentrations across a wide range on the formation of stable actin network bundles.While TEM provides a detailed yet narrow view of actin filament structure, confocal microscopy offers a broader perspective, crucial for understanding large-scale actin network organization. Additionally, the use of a flow system allows for the observation of actin network formation in a dynamic and continuous manner, surpassing the limitations of static batch conditions. This comprehensive approach not only highlights the role of Mg^{2+} in actin-ATP interactions and hydrolysis but also opens new avenues in disease modeling, therapeutic applications, and the development of artificial cell models, enhancing our understanding of cellular mechanisms.

Poster Presentation : **LIFE.P-165**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Dynamic behavior of DNA-gold nanoparticle assembly via interaction with enzymes

Jong wook Kim[*], **So-Jung Park**[*]

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DNA-functionalized gold nanoparticle (GNP) free-standing films were fabricated by a combination of layer-by-layer (LbL) self-assembly and plasmonic photothermal patterning. In order to maintain the structural stability of the film, covalent bonding through DNA T4 ligase was introduced and it was confirmed that the dynamic behavior of film is possible due to external stimuli such as temperature and salt concentration as well as the sequence recognition properties of DNA. We aim to induce dynamic behavior of the assembly through biomimetic stimulation based on the interaction between enzymes and DNA in this study. The results show that the enzyme-assisted dynamic behavior strategy can engineer dynamic behavior of DNA-GNP assemblies after their in vivo insertion.

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Poster Presentation : **LIFE.P-166**

Life Chemistry

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Crowder Effects on Biomolecular Phase Separation

<u>Hyun-Ah Jo</u>, Chan-Gyu Kim, Ha-Eun Kim, Jeong-Mo Choi[*]

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Liquid-liquid phase separation (LLPS) of biomolecules plays a vital role in several cellular activities. In a living cell, a dense assembly of large molecules such as proteins, RNA, and DNA facilitate a myriad of chemical reactions and interactions, and this state of molecular crowding significantly influences cellular biochemical and structural processes, including LLPS. Hence, crowding agents are utilized in typical in vitro LLPS experiments to replicate the crowded cellular environment. Despite this conceptual understanding, the molecular details regarding the role of crowding agents in LLPS have not been fully revealed. In this work, we utilized different crowding conditions to explore the effects of crowding agents on LLPS of multi-domain proteins. We observed the phase behavior of eYFP trimers using fluorescence microscopy in the presence of crowding agents, revealing conditions that resulted in distinct droplet formation. We also quantitatively determined the material properties of protein-rich phases, as a function of the crowding conditions. This study improves our understanding on the role of crowding agents in LLPS, which could help us design more effective phase separation experiment.

Poster Presentation : **LIFE.P-167**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

The Role of TAK1 and Nrf2 in Regulating Proliferation of Colon Cancer Cells with K-RAS Mutation

Seoyeon Park, Do-Hee Kim*, Sunghyun Hong, Hanbin Lim

Department of Chemistry, Kyonggi University, Korea

Transforming growth factor-β (TGF- β) - activated kinase 1 (TAK1, also known as MAP3K7) is a serine/threonine kinase in the mitogen-activated protein kinase (MAP3K) family. TAK1 can promote tumor cell survival/progression by modulation of apoptotic signaling and stress responses. By regulating the phosphorylation status and activities of transcription factors including AP-1 and NF-κB, TAK1 mediates inflammatory and prosurvival responses. TAK1 is a potential therapeutic target for cancers and inflammatory diseases. The object of this study is to evaluate the inhibitory effect of synthetic compounds on the TAK1 activity and to determine the molecular mechanism in colon cancer cells. Both TAK1 and Nrf2 expression were upregulated in colon cancer SW620 cells. We found that knockdown of TAK1 attenuated cell proliferation via inhibiting Nrf2-mediated SLC7A11 expression in colon cancer cell lines. We discovered novel acrylic acid derivatives, which were found to exhibit a potent inhibitory effect against TAK1. This compound showed excellent in vitro kinase activity for TAK1 and antiproliferative activity in various colon cancer cells. This compound may preferentially bind to the cysteine residue present in the active site of TAK1. When compared with (5Z)-7-oxozeaenol, known as a TAK1 inhibitor, a new synthetic compound induced stronger apoptotic effects, which was found to suppress Nrf2 signaling in colon cancer cells. Taken together, these findings suggest TAK1 inactivation through cysteine modification as a potential therapeutic approach for the treatment of colon cancer.Keywords: TAK1, Colon cancer, Nrf2, SLC7A11, Anti-proliferative activity

Poster Presentation : **LIFE.P-168**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Altering cell-surface receptors for the purpose of identifying receptor-specific glycosylation.

Chang-hee Lee, Injae Shin[*]

Department of Chemistry, Yonsei University, Korea

The epidermal growth factor receptor (EGFR), a glycoprotein situated on the cell surface, primarily functions in cell proliferation. Elevated levels of EGFR are closely linked with various tumor developments. Moreover, the glycans attached to EGFR are recognized to influence its response to epidermal growth factor (EGF) stimulation. Recognizing the physiological significance of EGFR, we created fluorescently tagged EGFR (EGFR128-AZDye 488) on cell membranes using genetic code expansion and bioorthogonal chemistry techniques. Through this method, sialic acid residues on EGFR were specifically identified on live cell surfaces, with EGFR serving as a FRET donor and cellular glycans as a FRET acceptor labeled with rhodamine. These findings collectively indicate that fluorescently labeled EGFR stands as a valuable instrument for delving into EGFR's cellular functions.

Poster Presentation : **LIFE.P-169**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Engineering of cell-surface receptors to study receptor internalization

Chang-hee Lee, Sookil Park, Injae Shin*

Department of Chemistry, Yonsei University, Korea

The epidermal growth factor receptor (EGFR), a glycoprotein present on the cell surface, plays a primary role in cell proliferation. Increased levels of EGFR are closely related to various tumor development. Furthermore, the glycans bound to EGFR are known to regulate its response to epidermal growth factor (EGF) stimulation. Owing to the pathophysiological significance of EGFR, we constructed EGFR128-AZDye 488, a fluorescently labeled EGFR, on the plasma membrane using genetic code expansion and bioorthogonal chemistry techniques. EGFR128-AZDye 488 was utilized to investigate the time-dependent internalization of EGFR in live cells. Results indicated that inhibitors and antibodies of EGFR suppress its internalization induced by EGF, and that lectins recognizing EGFR glycans do not affect its uptake into cells. It was also found that EGFR lacking sialic acid or fucose residues is internalized more efficiently than the wild-type EGFR. In summary, these findings suggest that fluorescently labeled EGFR serves as a valuable tool for exploring the cellular functions of the EGFR.

Poster Presentation : **LIFE.P-170**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Engineering Liquid-Liquid Phase Separation of Multi-Domain Proteins

Ha-Eun Kim, Chan-Gyu Kim, Hyun-Ah Jo, Jeong-Mo Choi*

Department of Chemistry, Pusan National University, Korea

Recently, there has been a growing interest in the liquid-liquid phase separation (LLPS) of biomolecules. It is known that biomolecules inducing phase separation exhibit weak multivalent interactions among themselves. Multi-domain proteins, whose folded domains participate in weak interactions, are one of the archetypal examples. Leveraging our knowledge in LLPS, we have successfully designed and engineered a new protein system capable of undergoing LLPS. We designed trimers of yellow fluorescent proteins (YFPs) and investigated their LLPS behaviors. By comparing wildtype and mutants with varying binding affinities, we anticipated that the pattern of phase separation would manifest differently depending on the protein's binding affinity. Based on the saturation concentrations measured through fluorescence imaging and turbidity measurements, we observed a negative correlation between binding affinity and LLPS propensity. We believe that this work will serve as a stepping stone for the de novo design of LLPS systems.

Poster Presentation : **LIFE.P-171**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of modified elongation factor (EF-P) in vitro

Dohyun Kim, Joongoo Lee[*]

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

The elongation factor P (EF-P) is an enzyme that promotes peptide-bond formation and stabilizes peptidyl-transfer RNA in the catalytic center of the ribosome. In particular, this enzyme has been shown to enhance consecutive incorporation of prolines and other types of unnatural amino acids into a peptide chain as it alleviates ribosome stalling. In eukaryotic cells, EF-P is activated by post-translational modification enzymes EpmA, EpmB and EpmC, respectively. However, synthesizing post-translationally modified using the enzymes is laborious, limiting the use of its unique activity for biological applications. Here, we show direct synthesis of post-translationally modified functional EF-P in vitro without using the multiple enzymes. We chemically synthesize a set of unnatural amino acid (lysyl lysines: α-lysyl lysine and β-lysyl lysine enantiomers) residues that are only obtained by the sequential enzymatic reactions during the post-translational modification process in the cell. We use a ribozyme to charge the synthetic amino acids to a transfer RNA(tRNA) and incorporate them into a specific residue into the middle of EF-P. Further, we will demonstrate that cell-free systems supplemented with the EF-P enable the production of novel bio-based materials containing unnatural substrates that are not efficiently incorporated into a peptide chain by the ribosome.

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Poster Presentation : **LIFE.P-172**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Mutated ribosome-mediated biosynthesis of pyridazinone oligomers in vitro

Hyeongwoo Park

School of Interdisciplinary Bioscience & Bioengineering, Pohang University of Science and Technology, Korea

Peptides are attractive material because they are biocompatible and can be simply produced by cell or chemical synthesis. However, peptide bond has limitations that they are easily proteolyzed and have poor selectivity. To overcome the limitations, we created a new backbone, not a peptide bond, by using ribosome. Ribosome is known to make only peptide bonds. But we demonstrate ribosome-mediated polymerization of pyridazinone bonds via a cyclocondensation reaction between activated γ-keto and α-hydrazino ester monomers. In addition, we demonstrate the ribosome-catalyzed synthesis of peptide-hybrid oligomers composed of multiple sequence-defined alternating pyridazinone linkages. Our results highlight the plasticity of the ribosome's ancient bond-formation mechanism, expand the range of non-canonical polymeric backbones that can be synthesized by the ribosome, and open the door to new applications in synthetic biology. When the folding of FLN5 is altered on the Mutant Ribosome, the loop truncation mutants generate additional space, providing entropic freedom to the nascent FLN chain. Beta hairpin ribosomal protein loops within the exit tunnel play a role in restricting space, affecting the folding process. Therefore, by utilizing the mutated ribosome, it was possible to generate a greater amount of pyridazinone.

Poster Presentation : **LIFE.P-173**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

An orthogonal flexizyme recognizing a water-soluble leaving group

Haneul Jin, Joongoo Lee*

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

The Flexizyme system has expanded the types of substrates chargeable to tRNA, leading to remarkable growth in the field of in vitro incorporation of unnatural amino acid into proteins. However, the fundamental mechanism that requires converting the carboxylic acid moiety, which influences the solubility of amino acids, into an ester for activation has led to the limitation of charging substrates with low solubility. Additionally, despite the evolution of flexizymes to recognize specific leaving groups for activation, the lack of high orthogonality among them poses a challenge to the simultaneous charging of various substrates in the same space. To overcome these drawbacks, we synthesized (4-(hydroxymethyl)phenyl)phosphonic acid (HPP) by introducing a phosphonic acid to the benzene ring, dramatically improving solubility when used as an amino acid activating group. Furthermore, through SELEX, we discovered a flexizyme (pFx) capable of orthogonal recognition of HPP-activated amino acids. We predict that pFx, utilizing its orthogonality and the enhanced solubility of the leaving group HPP, not only has the potential to bring about a new expansion in the field of unnatural amino acid incorporation but could also spark in situ charging-TX-TL systems using flexizymes.

Poster Presentation : **LIFE.P-174**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Detection and Identification of Lysosomal β-hexosaminidases Using Near-Infrared (NIR) Fluorogenic Probes

Yujun Kim, Injae Shin[1,*]

Yonsei University, Korea

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

Lysosomal β-hexosaminidase catalyzes the hydrolysis of β-linked N-acetyl-D-hexosamine residues (βGlcNAc and βGalNAc) in glycoconjugates. Pathologically, inherited deficiencies in this enzyme caused by mutations lead to lethal lysosomal storage disorders such as Tay-Sachs disease (TSD) and Sandhoff disease (SD). Owing to pathophysiological significance of lysosomal β-hexosaminidase, we developed and applied a near-infrared (NIR) fluorogenic probe to selectively detect and identify lysosomal β-hexosaminidase. The probe was composed of (1) a GalNAc residue serving as a selective substrate for β-hexosaminidase, (2) an ethyl carbamate-containing NIR fluorophore for fluorescence labeling of the enzyme, and (3) an alkyne tag for click reaction to facilitate isolation of the labeled enzyme by affinity chromatography. The intact probe was non-fluorescent. However, when the βGalNAc moiety was cleaved from the probe by β-hexosaminidase, ethyl carbamate was liberated from the NIR fluorophore. The quinone methide intermediate formed in this manner then reacted with a nucleophilic site in the side chain of an amino acid(s) of the enzyme. This process affords the selective imaging and identification of β-hexosaminidase. Details will be described in the presentation.

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Poster Presentation : **LIFE.P-175**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Read-across Approach for Developmental Toxicity Assessment: A Case Study with Dibutyl Phthalate

Sihoon Lee, Han Bin Oh[1,*]

Chemistry, Sogang University, Korea

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

In efforts to overcome the economic and ethical issues associated with animal testing, alternative methodologies for risk assessment have been extensively devised. To support the new approach methodology, a read-across approach is an in silico method to fill data gaps by leveraging chemical, biological, and toxicological data from analogues, which can be integrated into next-generation risk assessment frameworks. This study describes the process of evaluating the developmental toxicity of Dibutyl Phthalate using the read-across method. The identification of analogues for Dibutyl Phthalate was performed by defining the Structure similarity profiler in the OECD QSAR Toolbox. To assess the mechanical complexity of developmental toxicity, similarity evaluations of Dibutyl Phthalates and their analogues were undertaken in the following four categories: 1) evaluation of physicochemical property's similarity, 2) evaluation of toxicokinetic similarity, including ADME, 3) evaluation of toxicodynamic similarity, and 4) evaluation of bioactivity similarity through High-throughput screening(HTS) assays from ToxCast. These findings demonstrate that the process of analyzing the developmental toxicity of Dibutyl Phthalate using the Read-across methodology can be presented as a utilized case study for regulatory decision-making.

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Poster Presentation : **LIFE.P-176**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

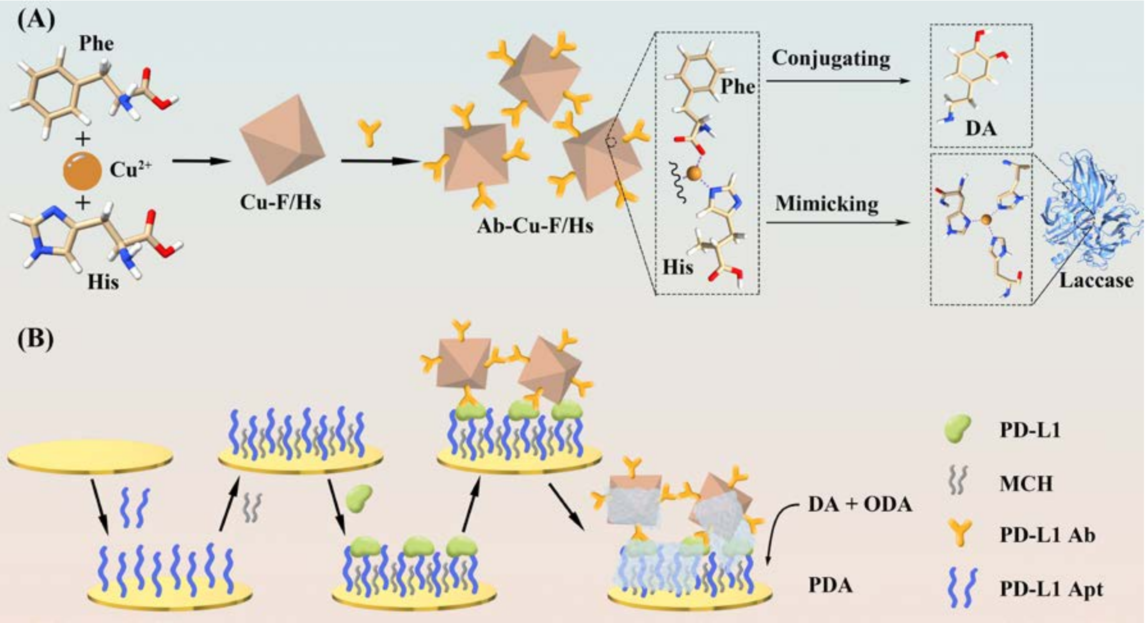
Laccase-inspired bi-amino acid MOFs with high substrate affinity: Catalytic deposition induced “signal-down” electrochemical response towards PD-L1

Xiaojun Hu[*], Jaebeom Lee[1,*]

Department of Chemistry, Research Institute of Materials Chemistry, China

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

A dual-ligand Cu-MOFs (Cu-F/Hs) based on phenylalanine (Phe) and histidine (His) was innovatively constructed with enhanced catalytic property. Among them, Phe can interact with the dopamine (DA) to enhance the substrate affinity. Meanwhile, the coordination of His with copper ions was inspired by the active site structure of natural laccase to improve the catalytic activity. The Km value of Cu-F/Hs was 0.14 times of laccase, indicating a high affinity for the catalytic substrate DA. Accordingly, a sensitive sensor for PD-L1 detection was designed by using Cu-F/Hs, which can catalyze DA to form polydopamine films deposited on the electrode surface with good electrical conductivity, thereby contributing a “signal-down” electrochemical response with a double signal enhancement. The detection limit was 0.12 ng/mL in the detection range of 0.5 – 200 ng/mL. This work provided a new and simple way to synthesize MOFs with high substrate affinity and efficient activity, and a general signal amplification strategy induced by the catalytic deposition.


(A)
Phe
+
Cu2+
+
His
Cu-F/Hs
Ab-Cu-F/Hs
Phe
His
Conjugating
Mimicking
DA
Laccase
(B)
DA + ODA
PDA
PD-L1
MCH
PD-L1 Ab
PD-L1 Apt

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Poster Presentation : **LIFE.P-177**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

DOM: *Dual Optical Mapping* Combining Sequence-Specific Markers and A/T Frequency-Dependent Profiles

Jaeyoung Bae, Kyubong Jo*

Department of Chemistry, Sogang University, Korea

We introduce Dual Optical Mapping (DOM), a method that combines sequence-specific barcode-like markers with AT frequency profiles. Optical Mapping has traditionally used barcodes generated by sequence-specific enzymes such as restriction endonucleases, nickases, or methyltransferases. This approach has been commercialized for genomic science applications. In addition, several AT frequency-dependent profiling approaches have been developed, including our prior work on fluorochrome-labelled pyrrole-octamers. Understanding the complementary capabilities of these methods, we conceived DOM, combining sequence-specific barcodes with AT frequency profiles. For efficient alignments, we developed a software tool, DOM.py, that automatically calculates cross-correlation values while considering DNA stretching. This program includes two established optical mapping tools, Maligner and OMBlast, facilitating a comparison of our cross-correlation results. To construct a precise reference map, we performed a computer simulation, postulating that a pyrrole-octamer would preclude neighbouring bindings when bound to an AT-specific site. Using DOM.py with a simulated reference map, we applied DOM to the E. coli genome (4.6 Mbp) as a representative model. We isolated single-molecule images of 182 DNA molecules exceeding 100 kb in length, with 178 of them aligning to the genome in 5.9× coverage. This remarkable alignment rate (98%) demonstrates our confidence in the capability of DOM to align single-molecule DNA images with reference genomes. Consequently, this work highlights DOM's potential for accurately interpreting single-molecule optical mapping DNA images.

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Poster Presentation : **LIFE.P-178**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Sequence-based peptide design for the α-Synuclein aggregation inhibition

SangHun Woo, Je Young Yoo, YouRa Lee, Young-Hee Shin[*]

Chemical Engineering & Biotechnology, Tech University of Korea, Korea

Neurodegenerative diseases such as Alzheimer's disease, Parkinson's disease, and Huntington's disease have emerged as a serious social problem in the aging population, requiring urgent strategies for treatment and prevention. Among these diseases, Parkinson's disease (PD), which is characterized by cognitive and motor disorders, is noticeable, and α-Syn protein aggregates are observed in the brain neural circuits of affected individuals. A recent study actively explored the "brain-gut axis" to suggest that brain neuron health is affected by the intestinal microbiota. In addition, according to the report, α-Syn aggregation can be promoted through the interaction of the intestinal microbiota environment, specifically Csg-A, a membrane protein Curli subunit of E. coli, with intestinal secretory cells, affecting α-Syn aggregation through the intestinal nervous system. Against this background, the present study seeks to develop a therapeutic approach for Parkinson's disease by developing a peptide derived from the chaperone protein Csg-C of E. coli to disrupt the interaction of Csg-A with α-Syn, thereby inhibiting amyloid formation and aggregation.

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Poster Presentation : **LIFE.P-179**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Developing Antibifilm α/β/γ Peptides with Enhanced Resistance to Degradation

Jihoo Jung, HyeonUk An, Young-Hee Shin*

Chemical Engineering & Biotechnology, Tech University of Korea, Korea

Biofilm, a cluster of microorganisms adhering to surfaces, poses significant challenges in healthcare settings due to its association with infectious diseases. Traditional antibiotic treatments struggle to penetrate biofilm matrices effectively, leading to antibiotic resistance. As an alternative, antimicrobial peptides (AMPs) have garnered attention for their broad-spectrum activity. However, AMPs like LL37 face limitations due to rapid degradation in vivo. This study aimed to enhance AMP stability by substituting LL37 sequences with β and γ amino acids. Candidate sequences were designed and evaluated for antimicrobial efficacy against S. mutans. The stability against protein-degrading enzymes was assessed, revealing FF16βγ with significantly prolonged half-life compared to FK16. FF16βγ demonstrated antibacterial efficacy comparable to FK16, indicating potential as a biofilm remover. Further validation is required to confirm the modeled peptides' structural integrity and biofilm removal effectiveness. Overall, incorporating β and γ amino acids shows promise in overcoming AMP stability challenges

Poster Presentation : **LIFE.P-180**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Bioorthogonal Imaging Probe for Sting Protein in Live Cell and Fixed Tissue

Wonjin Park, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Stimulator of interferon genes (STING) is an endoplasmic reticulum membrane protein that plays a vitalrole in innate immunity. In this study, we report a new bioorthogonal chemical probe derived from apreviously reported synthetic STING agonist by properly installing a trans-cyclooctene group withoutperturbation of the efficacy of the ligand. The probe is employed to investigate localization dynamics ofSTING in live cultured human cells and fixed mouse brain tissues. We showed that an optimized labelingstrategy employing the probe and tetrazine-silicon rhodamine fluorophore conjugates in a stepwise mannerenables the successful tracking of STING in live cells using fluorescence microscopy. Overall, ourbioorthogonal approach using the probe will facilitate in-depth investigations of intricate mechanismsassociated with STING.

Poster Presentation : **LIFE.P-181**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Spatiotemporal Control of Antibody-Drug Conjugates using STRIC (Stimulus TRIggered Cleavage) Technology

Jeonghyun Lee, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Antibody-drug conjugates (ADCs) have recently highlighted for cancer treatment due to their highly specific target recognition. In traditional ADCs, however, payloads are released after internalization into cancer cell, resulting side effects that activate against healthy cells. To address this issue, we envisioned a novel strategy, STRIC (Stimulus TRIggered Cleavage), to release payloads extracellularly using cleavable linkers. In this study, we synthesized biorthogonal pairs such as cleavable TCO linkers and a library of tetrazine small molecules to develop an improved ADC platform that can allow the payload release in spatiotemporal fashion.

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Poster Presentation : **LIFE.P-182**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of spatial control of tetrazine ligation

Lee Minju, Eunha Kim[*]

Department of Molecular Science and Technology, Ajou University, Korea

Tetrazine ligation techniques have evolved into a versatile toolset for bioconjugation, offering numerous applications. Despite their broad utility, highly reactive tetrazines may encounter off-target reactivity, presenting challenges in achieving cell-selective bioconjugation.In our study, we synthesized tetrazines with faster kinetics than previously reported, discovering that protecting certain functional groups could impede the TCO and release reactions. Leveraging these results, we envisioned into enzyme-initiated tetrazine uncaging, a method that enables controlled release of reactive tetrazines through enzymes overexpressed in certain cell types.Our novel design involved linking tetrazine to a glucuronide moiety, serving dual roles as a recognition element for cancer-associated β-glucuronidase and a caging group to modulate tetrazine activity. Through this approach, we successfully demonstrated cell-selective spatial control of tetrazine ligation.

Poster Presentation : **LIFE.P-183**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

New strategy of immunofluorescence cell imaging based on “click to release” mechanism

Jeonghyun Lee, Eunha Kim[1,*]

department of molecular science and technology, Ajou University, Korea

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

Various cell imaging methods have been utilized so far, but there are few methods for observing living cells in a multiplexed manner over time. Here, we present a new method that allows the removal of fluorescent signals at desired times. This method is based on click chemistry and is characterized by bioorthogonality, rapid reaction, and clear removal. We have validated this method by using several types of antibodies and targeting different cells. We expect this method to be applied to various biological systems.

Poster Presentation : **LIFE.P-184**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Hyaluronic acid nanoparticles as a topical agent for treating psoriasis

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Ajou University, Korea

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

Conventional topical approaches aimed at addressing psoriasis have been presented as an alternative; however, existing challenges such as low skin-penetrating efficiency and off-target adverse effects persist. In our investigation, we have established the viability of Hyaluronic Acid Nanoparticles (HA-NPs) as a topical therapeutic option for treating psoriasis. Our findings indicate that HA-NPs exhibit robust therapeutic efficacy against psoriasis-like skin dermatitis in a size-dependent manner. This efficacy is attributed to the suppression of innate immune responses and the restoration of skin barrier function, all achieved without displaying overt signs of toxicity. The therapeutic impact of HA-NPs on psoriasis-like skin dermatitis is attributed to the outermost hydrophilic Hyaluronic Acid (HA) shell layer of the nanoparticles. Importantly, this effect is independent of the molecular weight of HA and the hydrophobic moiety. Notably, the therapeutic efficacy of HA-NPs is comparable to that of other conventional psoriasis therapeutics widely employed in clinical settings. In summary, our study suggests that HA-NPs hold significant potential as a topical nanomedicine for effectively and safely treating psoriasis.

Poster Presentation : **LIFE.P-185**
Life Chemistry
Exhibition Hall 2 FRI 11:00~13:00

DNA aptamer-conjugated lipid nanoparticle for targeted PTEN mRNA delivery to prostate cancer cells

Jong Sam Lee, Dong-Eun Kim*

Department of Bioscience and Biotechnology, Konkuk University, Korea

The use of messenger RNA (mRNA) as a cancer vaccine and gene therapy requires targeted vehicle delivery to the site of disease. Here, we designed a mRNA-encapsulating lipid nanoparticle (LNP) conjugated with anti-programmed death-ligand 1 (PD-L1) DNA aptamer that delivers mRNA encoding a tumor suppressor gene, namely phosphatase and tensin homolog (PTEN), to castration-resistant prostate cancer (CRPC) cells expressing PD-L1 on the cell surface. The DNA aptamer-conjugated LNP-based mRNA delivery system (Apt-LNP[PTEN mRNA]) mediated efficient mRNA delivery and transfection in CRPC cells than LNPs without targeting ligands. Cancer-targeted PTEN mRNA achieved significantly higher PTEN expression via aptamer-mediated endocytosis in target cancer cells compared with non-targeted LNP delivery, resulting in significant downregulation of AKT phosphorylation. This enhanced PI3/AKT pathway regulation, and in turn reduced cell migration after two days along with a 70% decrease in cell viability, leading to effective apoptotic cell death. In a CRPC xenograft model, Apt-LNP[PTEN mRNA] led to an approximate 60% reduction in tumor growth, which was attributable to the effective PTEN restoration and PI3/AKT signaling pathway regulation. PTEN expression was significantly enhanced in CRPC tumor tissues, which abolished cancer cell tumorigenicity. These findings demonstrated the potential of Apt-LNPs for targeted mRNA delivery to cancer cells, thus providing a promising tool for targeted mRNA delivery to a range of cancers and tissues using a conventional LNP systems.

Poster Presentation : **LIFE.P-186**

Life Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Targeted delivery of anticancer drugs and siRNA to leukemic cells with DNA aptamer-conjugated liposome

Hyesoo Jin, Dong-Eun Kim*

Department of Bioscience and Biotechnology, Konkuk University, Korea

Acute myeloid leukemia (AML) is a hematologic malignancy characterized by the rapid proliferation of abnormal myeloid cells in the bone marrow and peripheral blood. Despite conventional treatment with chemotherapy drugs such as daunorubicin (DNR) and cytarabine (CYT), AML treatment remains challenging due to the development of drug resistance and the presence of leukemic cells in the bloodstream. Additionally, chemotherapy using DNR even induced immune suppression by increasing levels of indoleamine 2,3-dioxygenase-1 (IDO1). In this study, we developed a combination of DNA-conjugated liposomal nanoparticles to accomplish effective targeted delivery of anticancer drugs (DNR & CYT) as well as IDO1 siRNA into AML cells (OCl-AML2) in vitro. Anticancer drugs DNR & CYT and IDO1 siRNA was encapsulated into neutral liposome and cationic liposome harboring cationic phospholipid (DOTAP), respectively, which are conjugated with two DNA aptamers targeting the surface antigen of leukemic cell; CD33 and Nucleolin. IDO1 siRNA is a potential therapeutic approach for AML, as it can reduce IDO1 levels and subsequently enhance the effectiveness of chemotherapy by mitigating immune suppression. Leukemic cell-targeting efficacy of the aptamer-conjugated liposomes were tested in AML cells and revealed that presence of the DNA aptamers on liposomes enhanced efficiency of liposomal delivery by 24-fold as compared to the plain liposome without DNA aptamers. Thus, our DNA-conjugated liposomal nanoparticles will be useful targeted delivery of combined anticancer reagents such as DNR & CYT and IDO1 siRNA to leukemic cells without risk of nonspecific side effects of chemotherapeutics.

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Poster Presentation : **LIFE.P-187**
Life Chemistry
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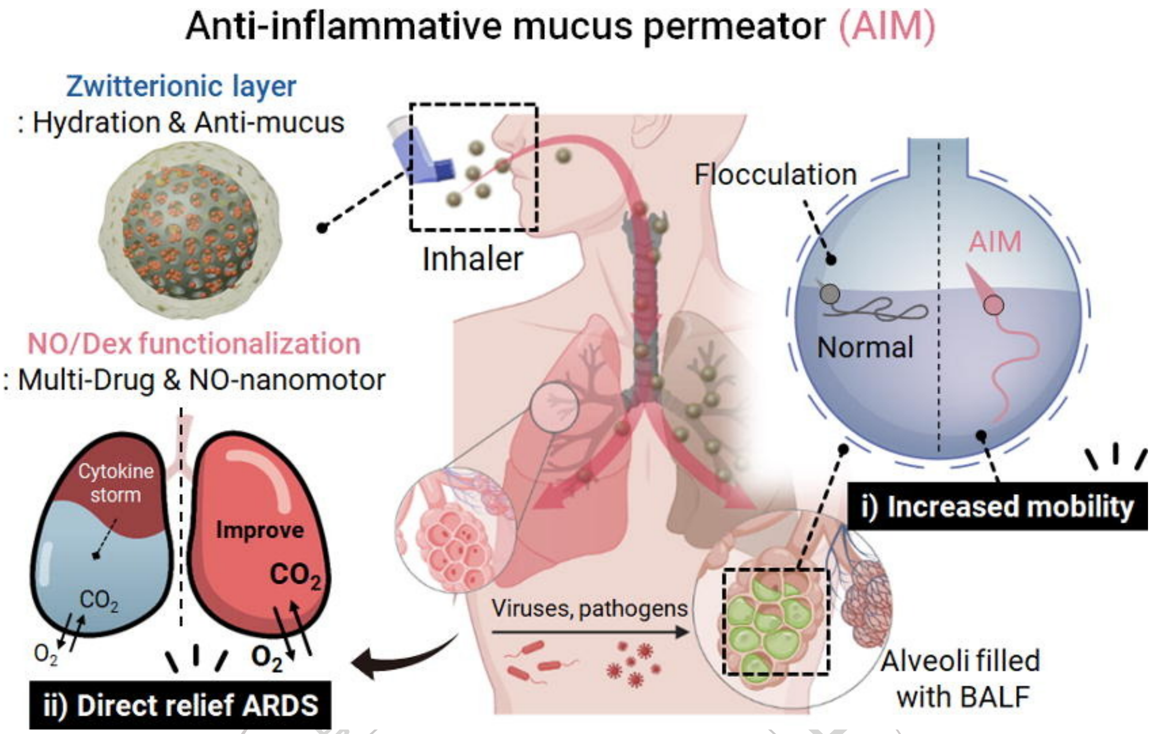
Zwitterionic nanocomplexes aided by Nitric Oxide nanomotors utilizing mucus-walking mechanism to offer a synergistic treatment approach for ARDS

Hye-Jin Lee, **Wonhwa Lee***

Department of Chemistry, Sungkyunkwan University, Korea

Among patients who suffer from lung-related disability, acute respiratory distress syndrome (ARDS) is one of the diseases with the significant mortality rate and the main cause is the interference in pulmonary drug delivery by accumulated bronchoalveolar lavage fluid (BALF) in the alveolar region. Here, a zwitterion-functionalized multi-drug nanocomplex (ZnC) capable of anti-mucociliary clearance was synthesized. Additionally, nitric oxide (NO) was functionalized with ZnC to fuel the mobility in the BALF through its role as a nanomotor as well as anti-inflammation. Subsequently, dexamethasone (Dex) was loaded and final product of anti-inflammatory mucus permeator (AIM) was introduced. By in situ tracking the AIM within the mucus-rich environment, the fueled mobility by NO and zwitterion was demonstrated. Notably, when AIM was inhaled by the in vivo ARDS model, there was an increase in the anti-inflammation effect due to the presence of ZnC as well as the synergy between NO and Dex, which recovered the pulmonary function of the model and increased survival rate.


Anti-inflammative mucus permeator (AIM)
Zwitterionic layer
: Hydration & Anti-mucus
NO/Dex functionalization
: Multi-Drug & NO-nanomotor
Inhaler
Flocculation
AIM
Normal
i) Increased mobility
Cytokine storm
Improve
CO_2
CO_2
O_2
O_2
ii) Direct relief ARDS
Viruses, pathogens
Alveoli filled with BALF

Poster Presentation : **ORGN.P-188**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Photoredox catalysis/initiation of substituted fluoresceins under visible light

Hoyun Kim, Fisayo Jegede[1], Dogyeong Lee[1], JungKyu Lee[1,*]

Chemistry, Kyungpook National University, Korea

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

We demonstrated the effects of substituents in fluorescein on the photoredox catalytic performance under visible light. For the systematic investigation, the phenyl ring of fluorescein was substituted with six different functional groups (i.e., amine, amide, isothiocyanate, aminomethyl, bromo, or nitro group) at the 5- or 6-position. The fluorescein derivatives were carefully characterized through photophysical and electrochemical analyses. The substituent effects were estimated by comparing the photopolymerization of poly(ethylene glycol) diacrylate (PEGDA) and N-vinylpyrrolidone (VP) in the presence of triethanolamine (TEOA) under aerobic conditions to that of intact fluorescein. As a result, the amine and nitro groups exhibited the lowest performances, presumably due to intramolecular photoinduced electron transfer (PET) promoted by the strong electron push–pull effect. The others, representative moderate or weak deactivators and activators, exhibited inferior performances than intact fluorescein, presumably owing to the more negative ΔGPET values, resulting in a decreased rate of intermolecular PET. These results are crucial for understanding the structure–performance relationship and the development of visible-light photoredox catalysts with improved performance and functionality.

Poster Presentation : **ORGN.P-189**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

One-Pot Three-Component Reaction for the Synthesis of 3,4-Dihydroquinazolines and Quinazolin-4(*3H*)-ones

Yeong Shin Ji, So Won Youn*

Department of Chemistry, Hanyang University, Korea

The quinazoline structure is widely recognized as a key motif in bioactive molecules that exhibit a wide range of biological and pharmacological activities. Most of the synthetic routes suffer from the disadvantages of requiring multistep procedures, use of hazardous chemicals, high cost and safety concerns, which limit their practicality. Recently, our group has developed an efficient, metal-free, and mild one-pot reaction for the synthesis of diverse range of 3,4-dihydroquinazolines and quinazolin-4(*3H*)-ones. A domino three-component assembly reaction of arenediazonium salts, nitriles, and bifunctional aniline derivatives resulted in the formation of three different C-N bonds.

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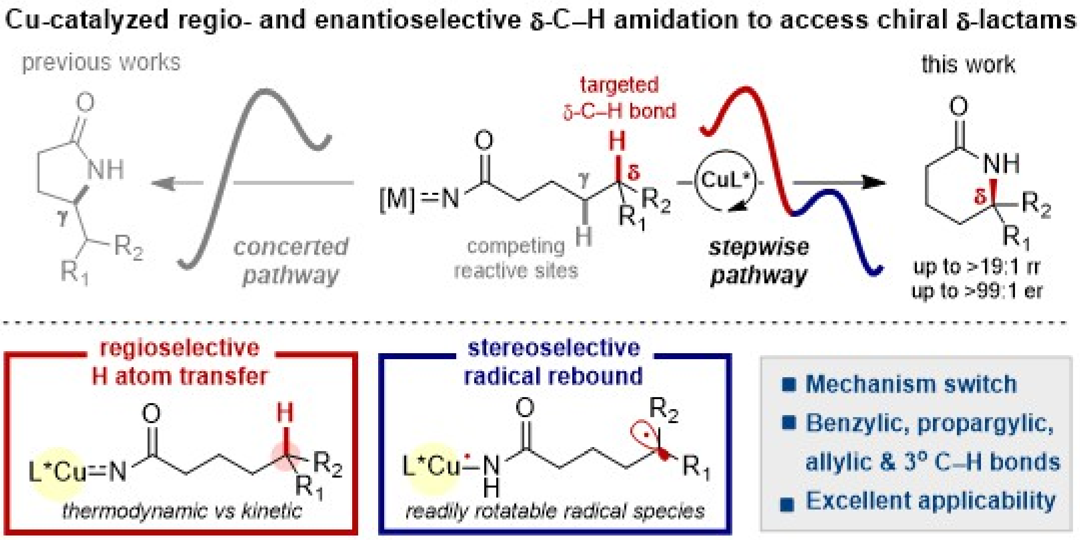
Poster Presentation : **ORGN.P-190**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Regio- and Enantioselective Catalytic δ-C–H Amidation of Dioxazolones Enabled by Open-Shell Copper-Nitrenoid Transfer

Suhyeon Kim, Sungwoo Hong, Sukbok Chang[1,*]

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

This study focuses on the critical task of controlling regio- and enantioselectivity in C–H functionalization reactions, which have significant synthetic applications. We present a novel approach for achieving asymmetric δ-C(sp^3)–H amidation catalysis of dioxazolones utilizing a Cu(I) precursor with a chiral bisoxazoline ligand, resulting in the synthesis of six-membered lactams with remarkable levels of regio- and enantioselectivity (up to >19:1 rr and >99:1 er). Through a comprehensive combination of experimental and computational mechanistic studies, we elucidate how the open-shell nature of the proposed Cu-nitrenoids facilitates regioselective hydrogen atom abstraction and subsequent enantiodetermining radical rebound of the resulting carbon radical intermediates. Moreover, we demonstrate the practical applications of this asymmetric cyclization method, including the diastereoselective introduction of additional functional groups into the chiral δ-lactam skeleton and the rapid synthesis of biorelevant azacyclic compounds.


Cu-catalyzed regio- and enantioselective δ-C–H amidation to access chiral δ-lactams
previous works
O
NH
γ
R$_2$
R$_1$
concerted pathway
targeted δ-C–H bond
H
δ
[M]=N
O
γ
H
R$_2$
R$_1$
competing reactive sites
CuL*
stepwise pathway
this work
O
NH
δ
R$_2$
R$_1$
up to >19:1 rr
up to >99:1 er
regioselective H atom transfer
L*Cu=N
O
H
R$_2$
R$_1$
thermodynamic vs kinetic
stereoselective radical rebound
L*Cu–N
H
O
R$_2$
R$_1$
readily rotatable radical species
Mechanism switch
Benzylic, propargylic, allylic & 3° C–H bonds
Excellent applicability

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **ORGN.P-191**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

One-Pot Conversion of D-ribose into Pyrrole Heterocyclic Platform Compounds-Synthesis of Lamellarin O Derivatives

Tang Ting, Sangho Koo[1,*]

Organic chemistry, Myungji University, China

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

Lamellarin O, a marine alkaloid characterized by its distinct and stable structure, exhibits a diverse spectrum of biological activities.This study presents an efficient synthesis of lamellarin O derivatives, utilizing the Delépine reaction,aminoketone with D-ribose conversion, and Suzuki-Miyaura coupling. Concurrently, a comprehensive exploration of the structural and functional relationships among substituents with varying electronic properties will be conducted, aiming to identify additional compounds with promising biological activities.

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Poster Presentation : **ORGN.P-192**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Effective synthesis of Grifolin exhibiting biological activity using 5-methylcyclohexane-1,3-dione.

Dabin Kim, Sangho Koo[1,*], Bo-ram Lim[2,*]

Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*
[2]*Bangmok College of General Education, Myungji University, Korea*

Grifolin is natural compound found in the mushroom, Albatrellus confluens, having biological effects such as antioxidant and anticancer properties. It prevents tumor formation at an early stage and suppresses the process of cancer cell proliferation and the metastasis through anti-angiogenic action. We have been studying the total synthesis of grifolin, which is based on combination of a resorcinol core and a farnesyl chain. The Fridel-craft alkylation has encountered challenges related to regiochemistry and cyclization. Our new proposal is to use 5-methylcyclohexane-1,3-dione instead of resorcinol to overcome these problems. Regarding this, O-alkylation and C-alkylation were studied, and the C-alkylation product was aromatized. Our study can demonstrate that this is an effective method to synthesize grifolin.

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Poster Presentation : **ORGN.P-193**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis and Analysis of Oxo-Carotenoids for Efficient Superoxide Radical Scavenging

Sangho Koo[*], Hansuk Lee[1], Bo-ram Lim[2,*]

Department of Chemistry, Myongji University, Korea

[1]*Chemistry, Myungji University, Korea*

[2]*Bangmok College of General Education, Myungji University, Korea*

Carotenoids, naturally occurring compounds in vegetables, fruits, and other plants, possess antioxidant properties that shield cells and tissues from oxidative stress. Their antioxidant activity lies in their reactivity towards reactive oxygen species (ROS), which can induce lipid oxidation, DNA mutations, protein defects, and other forms of oxidative damage. Oxo-carotenoids, particularly those containing conjugated carbonyl groups, exhibit effective scavenging of the superoxide radical, a type of ROS. These oxo-carotenoids are synthesized via aldol condensation between polyene dials and acetophenones. The synthesis of polyene dials employs the Horner-Wadsworth-Emmons olefination, a chemical extension method. To assess the antioxidant activity of oxo-carotenoids, standard radical scavenging assays using DPPH and ABTS radicals were conducted and compared with the results from the superoxide anionic radical assay.

Poster Presentation : **ORGN.P-194**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Apocarotenals of Phenolic Carotenoids for Superior Antioxidant Activities.

Yang Liu, Sangho Koo[1,*]

Myungji University, China

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

A series of para-phenolic carotenes 1 with ortho- and meta-substitutions and the corresponding apo-12´-carotenals 2 were synthesized utilizing the benzenesulfonyl protection method. The conjugated aldehyde group in apo-12´-carotenals 2 can enhance the conjugation effect of the para-phenolic radical with the polyene chains. Apo-12´-carotenals 2b and 2c without ortho-substituents exhibited superior antioxidant activities compared to their corresponding symmetrical carotenes 1 when comparaing β-carotene and apo-12´-β-carotenal in ABTS and DPPH radical scavenging assays.

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Poster Presentation : **ORGN.P-195**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Total synthetic method for Tetraphenyl-Substituted All-*E*-Carotenoids as Molecular wire

Chibeom Seo, Sangho Koo[1,*]

the chemistry department, Myungji University, Korea

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

Carotenoids containing phenyl substituents in the polyene chain not only enhance various electron-conducting abilities to the chain, but also provide chemical stability. We synthesized 9,9´,13´-tetraphenyl-substituted polyene chain of carotenoids and measure the conductivity of them. The synthetic method of tetraphenyl-substituted all-*E*-carotenes 1 was developed through the formations of tetraphenyl-substituted all-*E*-apocarotenedial 4. olefination of Wittig salt and all-*E*-apocarotenedials 4 provided tetraphenyl-substituted all-*E*-carotenes 1.In the same method as above, We also synthesized tetraphenyl-substituted all-*E*-carotene containing EDG and EWG at the para-position of phenyl substituents to study the effect of each group on the conductivity. EDG such as methyl ($-CH_3$) and methoxy ($-OCH_3$) increased the conductivity, while EWG groups such as bromine (-Br) decreased the conductivity.

Poster Presentation : **ORGN.P-196**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of diglycerides from natural compounds

Sangho Koo[*], JiSu Hong[1]

Department of Chemistry, Myongji University, Korea

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

Natural compounds play a vital role in various physiological activities such as antioxidant, antibacterial, skin regeneration, and skin brightening. These compounds are widely utilized as ingredients in cosmetics, food products, and pharmaceuticals.However, organic acids are highly toxic to the skin, while phenol compounds have poor skin penetration. To address these challenges, glycerol has been introduced, and diglycerides have been synthesized by combining different phenols and organic acids.Initially, 1,3-diglyceride is synthesized by adding epichlorohydrin to a phenolic compound and then combining it with an organic acid using a Bu4NBr catalyst. The utilization of 1,3-acetal-protected glycerol enables the formation of 2-esters of organic acids within glycerol. Subsequent deprotection of the acetal and 2-etherification lead to the production of 1,2-diglyceride.This synthetic method holds the potential to address existing issues and offers two functional properties.

Poster Presentation : **ORGN.P-197**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Palladium-Catalyzed S-Allylation of Vinyl Carbinols: A Highly Efficient Approach for Carotenoid Synthesis via Julia-Kocienski Olefination

Sangho Koo*, Aleksei Golikov

Department of Chemistry, Myongji University, Korea

An efficient and typically high-yielding method for palladium-catalyzed *S*-allylation utilizing 2-mercaptobenzathiazole of vinyl carbinols is described. The synthetic versatility of the resulting benzothiazole sulfides is exemplified through the efficient synthesis of carotenoids, including β- and ε-carotenes, and 9'-Z-phenyl-carotene via Julia-Kocienski olefination. Furthermore, the selective transformation of vinyl carbinols, rather than allylic acetates, enables the preparation of naturally occurring xanthophylls such as lutein, zeaxanthin, and isozeaxanthin.

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Poster Presentation : **ORGN.P-198**

Organic Chemistry

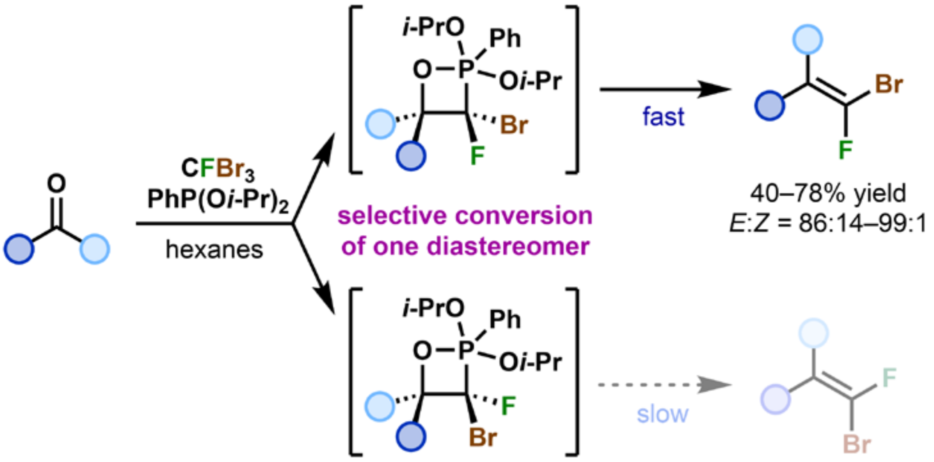
Exhibition Hall 2 FRI 11:00~13:00

A Stereoselective Synthesis of Geminal Bromofluoroalkenes Enabled by Kinetically Controlled Selective Conversion of Oxaphosphetane Intermediates

Jaeseong Jin, Jun-Ho Choi[*], Won-jin Chung[*]

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

Geminal bromofluoroalkenes are an important subclass of versatile organic interhalide, which can serve as useful synthetic precursors to monofluoroalkenes that are valuable amide group isosteres. Nonetheless, despite the vast advancement of olefination methodologies, the broadly applicable stereoselective synthesis remained elusive for geminal bromofluoroalkenes before our work. In particular, the seemingly straightforward Wittig-type approach with interhalogenated phosphorus ylide has been unsuccessful because of the difficulty in the diastereoselective oxaphosphetane formation. Herein, we describe a conceptually distinctive strategy, by which the stereoselectivity is gained via the selective decomposition of the oxaphosphetane intermediates. The suitably identified phosphorus(III) reagent and reaction medium enabled efficient kinetic differentiation, which was supported by NMR analysis and DFT calculation. Through our method, the highly diastereoselective synthesis of geminal *E*-bromofluoroalkenes was accomplished in one step for the first time. Furthermore, the generality was demonstrated by accommodating a wide range of readily available carbonyl compounds, including ketones and pharmaceutical substrates.



- new kinetic stereocontrol strategy
- quantitative ^{19}F NMR analysis
- DFT calculation
- high efficiency & excellent *E*-selectivity
- wide scope including ketones & pharmaceuticals
- mild reaction conditions

Poster Presentation : **ORGN.P-199**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

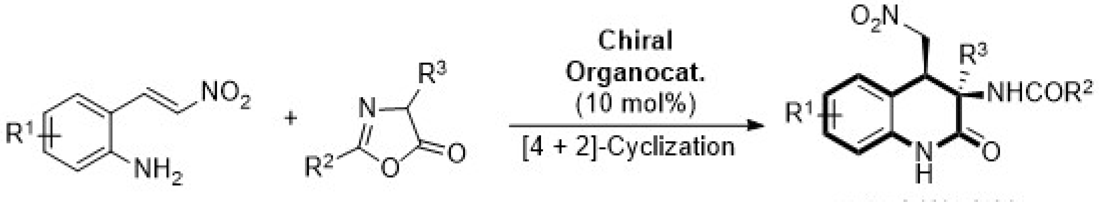
Enantioselective Synthesis of chiral 3,4-Dihydroquinolin-2-ones via organocatalytic [4+2]-Cyclization of 2-Amino-β-nitrostyrenes with Azlactones

Heebum Kim, Yeongju Kim[1], Sung-Gon Kim[*]

Department of Chemistry, Kyonggi University, Korea

[1]*Department of chemistry, Kyonggi University, Korea*

Dihydroquinolin-2-ones, recognized for their significant bioactive properties, feature a unique six-membered structure with nitrogen-containing heterocycles. A breakthrough method has been developed to synthesize enantioenriched 3,4-dihydroquinoline-2-one derivatives. This innovative approach utilizes an asymmetric [4+2]-cyclization process, combining 2-amino-β-nitrostyrenes with azlactones, and is facilitated by a bifunctional squaramide-based organocatalyst. This innovative approach has enabled the creation of novel chiral 3,4-dihydroquinoline-2-ones with complex structures, including chiral quaternary centers. The process is remarkably efficient, delivering high yields (up to 91%), excellent enantiomeric excess (up to 97% ee), and superior diastereoselectivity (up to 19:1 dr).



up to 91% yield
up to 97% ee, and 19:1 dr

Poster Presentation : **ORGN.P-200**

Organic Chemistry

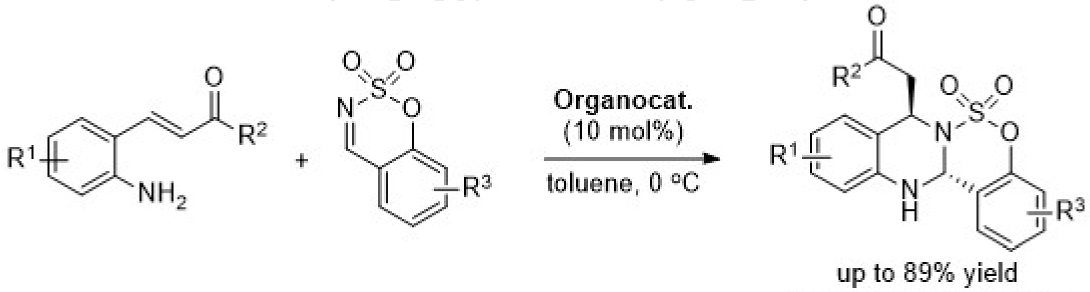
Exhibition Hall 2 FRI 11:00~13:00

Organocatalytic asymmetric [4+2]-cycloaddition of Cyclic N-Sulfimines with 2-Aminophenyl Enones

Yurim Kim, **Sung-Gon Kim***

Department of Chemistry, Kyonggi University, Korea

The structure of ring-fused aminals presents an intriguing scaffold in biologically active and pharmaceutically relevant compounds. A novel and highly efficient method for synthesizing chiral benzosulfamidate-fused tetrahydroquinazolines has been successfully developed. Through an organocatalytic asymmetric [4+2]-cycloaddition employing a squaramide-based catalyst, the enantioselective synthesis of chiral ring-fused tetrahydroquinazolines has been achieved with impressive results, including high yields and excellent enantio- and diastereoselectivities (yielding up to 89%, 94% ee, and >30:1 dr).



up to 89% yield
up to 94% ee, >30:1 dr

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Poster Presentation : **ORGN.P-201**

Organic Chemistry

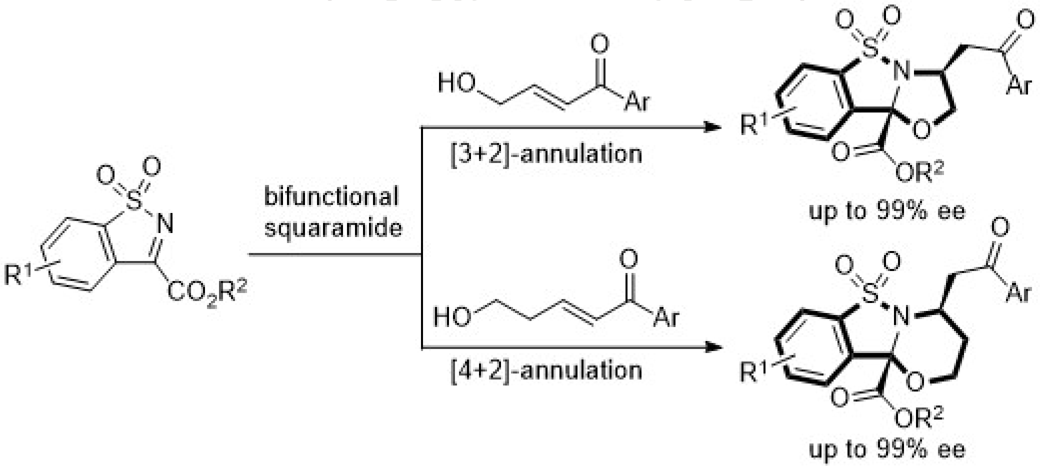
Exhibition Hall 2 FRI 11:00~13:00

Bifunctional Squaramide-Catalyzed Asymmetric Annulation of Cyclic N-Sulfonyl Ketimines with γ- or δ-Hydroxy-α,β-Unsaturated Ketones

Jiseon Yang, **Sung-Gon Kim**[*]

Department of Chemistry, Kyonggi University, Korea

A highly efficient enantioselective [3+2]/[4+2]-cycloaddition of cyclic N-sulfonyl ketimines with γ- or δ-hydroxy-α,β-unsaturated ketones has been developed. This innovative reaction employs an organocatalytic approach, utilizing a hydrogen-bonding bifunctional squaramide-based catalyst. The process enables precise synthesis of chiral polyheterotricyclic oxazolidines and 1,3-oxazinane derivatives, revealing intricate structures with incorporated chiral quaternary centers. Remarkably, this method delivers high yields and exceptional enantioselectivities and diastereoselectivities, achieving up to 99% yield, 99% ee, and >20:1 dr.



Poster Presentation : **ORGN.P-202**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

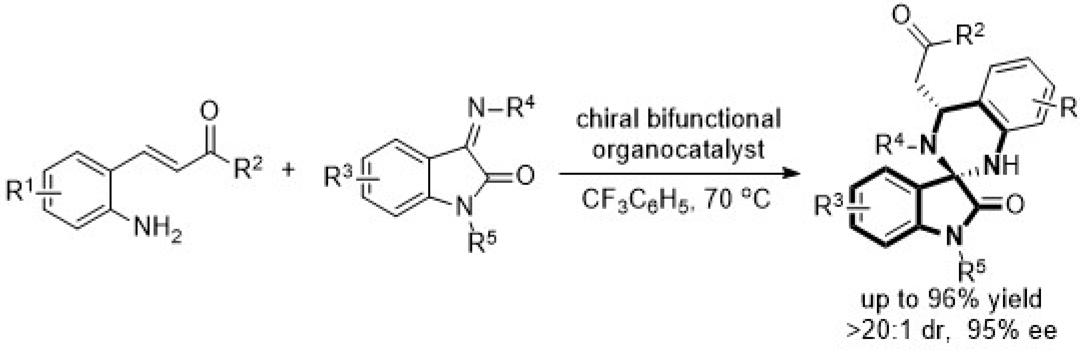
Organocatalytic Asymmetric [4+2]-Cycloaddition of 2-Aminophenyl Enones with Isatin-Derived Ketimines: Stereoselective Synthesis of Spirooxindole-Tetrahydroquinazolines

Jiwon Han, Sung-Gon Kim[1,*]

Kyonggi University, Korea

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

A novel method for the enantioselective synthesis of spiro N,N-heterocyclic oxindoles has been developed, employing asymmetric [4+2]-cycloadditions of 2-aminophenyl enones with isatin-derived ketimines. This method employs an organocatalytic approach, utilizing a bifunctional squaramide-based catalyst. It enables the precise synthesis of chiral spirooxindole-tetrahydroquinazolines with intricate structures, featuring chiral quaternary centers. This process achieves remarkable results, including high yields and exceptional levels of enantioselectivity and diastereoselectivity (up to 96% yield, 95% ee, and >20:1 dr).



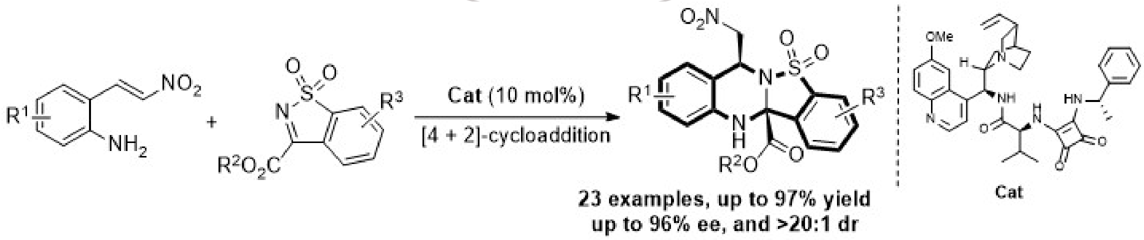
Poster Presentation : **ORGN.P-203**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Asymmetric Synthesis of Polycyclic Benzosultams via [4+2]-Cycloaddition of 2-Amino-β-nitrostyrenes with Cyclic N-Sulfonyl Ketimines

Yoseop Kim, Jiwon Han[1], Sung-Gon Kim*

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

A highly efficient enantioselective [4+2]-cycloaddition of 2-amino-β-nitrostyrenes with cyclic N-sulfonyl ketimines has been developed. This reaction utilizes an organocatalytic approach, employing a multiple hydrogen-bonding bifunctional squaramide-based catalyst. The process allows for the precise synthesis of chiral polycyclic benzosultams, showcasing intricate structures that incorporate chiral quaternary centers. Noteworthy outcomes of this method include high yields and excellent enantioselectivities and diastereoselectivities (up to 97% yield, 96% ee, and >20:1 dr).



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Poster Presentation : **ORGN.P-204**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Design of solvent ratio for highly stable metal oxide slurry systems and robust dielectric sheets

Jung Jin Park, Jong Ho Lee*

MLCC Process Architecture Lab, Samsung Electro-Mechanics, Korea

To fabricate high-end MLCC with thin dielectric layers, there is a pressing need to develop a technology that ensures the dispersion stability of nanoparticles and the mechanical strength of dielectric sheets. The stability of the slurry with oxide particles and defects in the dielectric sheet are determined by the solubility of the organic materials in solvent. Here, we investigate the solubility of binders with various solvent ratios. Thin sheets show different chemical and mechanical properties due to their solubility difference. We establish the design rule for solvent ratios and apply a new solvent ratio to increase solubility of binder. This results in exceptional dispersion stability and sheet strength, which are necessary for the development of ultra-thin dielectric sheets.

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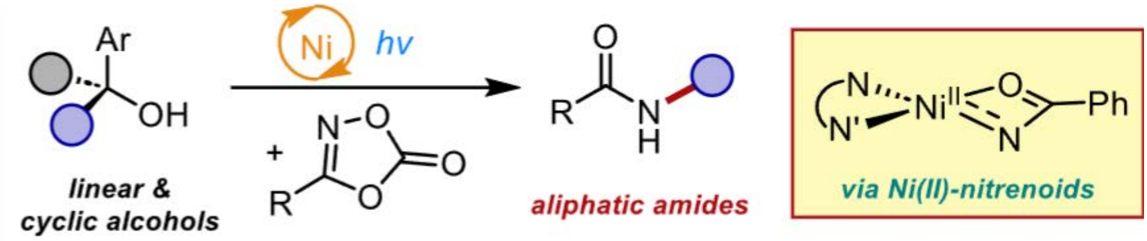
Poster Presentation : **ORGN.P-205**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Amidative *β*-Scission of Alcohols Enabled by Dual Catalysis of Photoredox Proton-Coupled Electron Transfer and Inner-Sphere Ni-Nitrenoid Transfer

Hyeyun Keum, **Sukbok Chang**[1,*]

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

The photoredox/Ni dual catalysis emerges as a promising strategy for facilitating unconventional C−heteroatom bond formation. Despite notable progress achieved with this system, intermolecular $C(sp^3)-N$ bond formation has been relatively underdeveloped due to the difficulty in $C(sp^3)-N$ reductive elimination. Herein, we present a new mechanistic approach that utilizes dioxazolones as the Ni(II)-nitrenoid precursor to capture carbon-centered radicals by merging proton-coupled electron transfer (PCET) with nickel catalysis, thus forming synthetically versatile *N*-alkyl amides using alcohols. Based on mechanistic investigations, the involvement of (*κ*2-N,O)Ni(II)-nitrenoid species was proposed to capture photoredox PCET-induced alkyl radicals, thereby playing a pivotal role to enable the $C(sp^3)-N$ bond formation.



- First example of PCET/Ni-catalyzed *amidative β-scission* using alcohols
- A Merger of *photoredox PCET and Ni-nitrenoid transfer*
- Mechanistic investigation of the *$C(sp^3)$–N bond formation process*

Poster Presentation : **ORGN.P-206**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Catalytic Asymmetric Formal C-C Bond Insertion Reaction: Synthesis of Acyclic All-Carbon Quaternary Stereocenters

Hye-Min Jeong, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

The enantioselective synthesis of all-carbon quaternary stereocenters is crucial in organic chemistry for pharmaceutical applications. Although cyclic systems have been extensively studied for the construction of all-carbon quaternary stereocenters, the exploration of acyclic systems in this context has remained largely unexplored. We present a novel method for the synthesis of chiral acyclic α-quaternary-beta-keto esters using aldehydes and alkyl diazo compounds. In the presence of a chiral oxazaborolidinium ion (COBI) catalyst, the enantioselective formal insertion reactions afforded chiral α-alkyl-α-formyl-β-ketoesters in high yields (up to 97%) with excellent enantioselectivities (up to >99%). A proposed mechanism and DFT calculations elucidate the observed stereochemistry. This reaction will show promising utility in various other challenging chemical reactions and complex medicinal intermediates.

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Poster Presentation : **ORGN.P-207**

Organic Chemistry

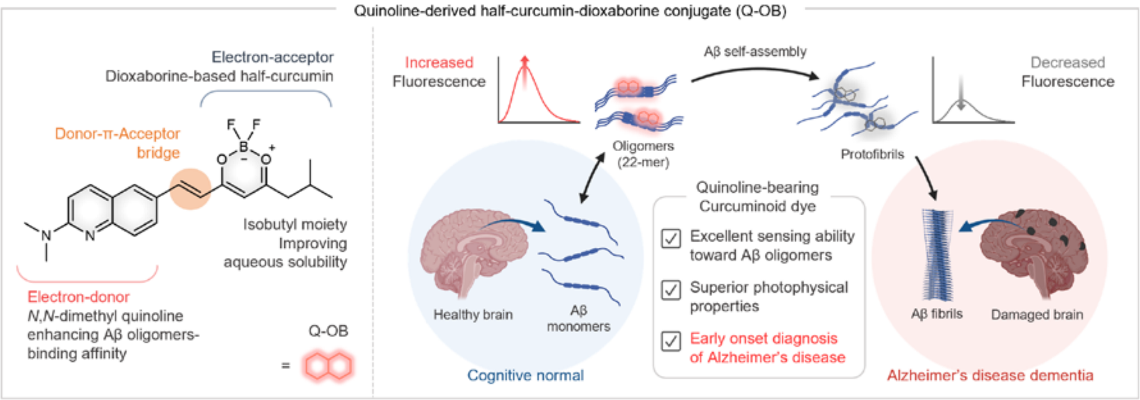
Exhibition Hall 2 FRI 11:00~13:00

Pioneering the early diagnosis of Alzheimer’s disease: Amyloid-β oligomers-sensing probe in patients’ cerebrospinal fluid

Jusung An, Jungryun Kim, Jaewon Kim, Qihang Ding, Hyeonji Rha, Eunji Kim, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Amyloid-β (Aβ) oligomers play a crucial role in the early stages of Alzheimer's disease (AD). In this study, a fluorescent probe based on quinoline-derived half-curcumin-dioxaborine (Q-OB) was developed specifically to detect Aβ oligomers. This was achieved by finely tailoring the hydrophobicity of the biannulate donor motifs within a donor-π-acceptor structure. Q-OB probe demonstrates significant efficacy in the real-time observation of Aβ oligomer formation during the process of amyloid fibril formation in vitro. Furthermore, this approach was utilized to perform fluorometric analysis of Aβ oligomerization kinetics in the cerebrospinal fluid (CSF) of patients with AD. The fluorescence intensity changes in the CSF of AD patients were quantitatively measured, showing a notable difference in the log (I/I_0) values of 0.34 ± 0.13 (cognitive normal), 0.15 ± 0.12 (mild cognitive impairment), and 0.14 ± 0.10 (AD dementia), which assists in identifying different stages within the AD continuum for the early diagnosis of AD. These findings underscore the capability of this method to enhance existing preclinical diagnostic platforms for early-stage AD, contributing to the interruption of its pathological progression and facilitating the formulation of targeted treatment approaches.


Quinoline-derived half-curcumin-dioxaborine conjugate (Q-OB)
Electron-acceptor
Dioxaborine-based half-curcumin
Donor-π-Acceptor
bridge
F F
B
O O
N
N
Isobutyl moiety
Improving
aqueous solubility
Electron-donor
N,N-dimethyl quinoline
enhancing Aβ oligomers-
binding affinity
Q-OB
=
Increased
Fluorescence
Aβ self-assembly
Decreased
Fluorescence
Oligomers
(22-mer)
Protofibrils
Quinoline-bearing
Curcuminoid dye
☑ Excellent sensing ability toward Aβ oligomers
☑ Superior photophysical properties
☑ Early onset diagnosis of Alzheimer's disease
Healthy brain
Aβ
monomers
Cognitive normal
Aβ fibrils
Damaged brain
Alzheimer's disease dementia

Poster Presentation : **ORGN.P-208**

Organic Chemistry

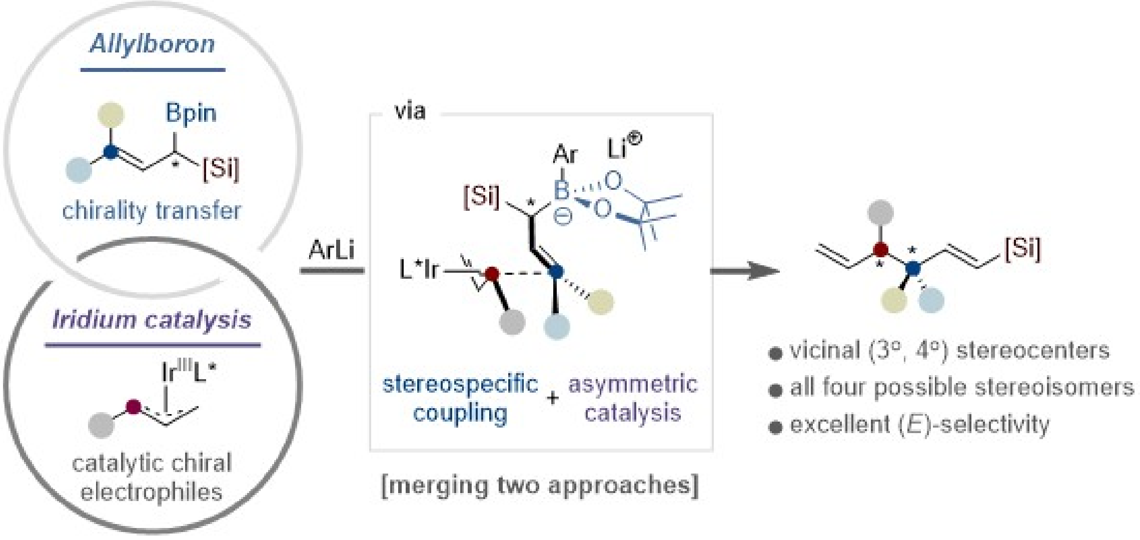
Exhibition Hall 2 FRI 11:00~13:00

Creation of Contiguous Tertiary and All-Carbon Quaternary Stereocenters through Stereospecific and Stereodivergent Allyl-Allyl Coupling

Yongsuk Jung, Seung Hwan Cho*

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

Organic synthesis has witnessed significant advancements in the development of efficient methods for precisely and reliably synthesizing complex enantioenriched molecules. Enantioenriched allylboronate esters are valuable synthetic intermediates in organic chemistry because of their ability to undergo highly regioselective and stereospecific coupling with a wide range of electrophiles.Herein, we demonstrate an iridium-catalyzed highly stereospecific and stereodivergent allyl-allyl coupling between branched allyl carbonates and α-silyl-γ,γ-dialkyl allylboronate esters. When 3,5-$(CF_3)_2$-phenyllithium was used as an activator of the boron group of α-silyl-γ,γ-dialkyl allylboronate esters, the enantioenriched (*E*)-1-silyl-substituted 1,5-dienes bearing a tertiary stereocenter adjacent to the all-carbon quaternary center are obtained. Notably, this approach allows access to all four possible stereoisomers by permuting the chirality of the employing α-silyl-γ,γ-dialkyl allylboronate esters and ligands. Further synthetic elaborations of the obtained enantioenriched (*E*)-1-silyl-substituted 1,5-dienes are also illustrated to afford a range of enantioenriched molecules.


Allylboron
Bpin
[Si]
chirality transfer
Iridium catalysis
Ir^{III}L*
catalytic chiral electrophiles
ArLi
via
Ar
Li$^{\oplus}$
[Si]
B
O
O
⊖
L*Ir
stereospecific coupling
+
asymmetric catalysis
[merging two approaches]
[Si]
vicinal (3°, 4°) stereocenters
all four possible stereoisomers
excellent (E)-selectivity

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Poster Presentation : **ORGN.P-209**

Organic Chemistry

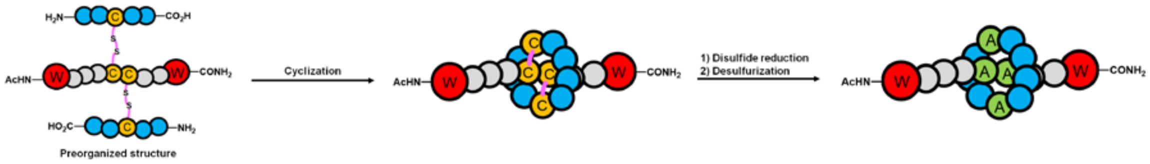
Exhibition Hall 2 FRI 11:00~13:00

Design & synthesis of peptide [2]rotaxane comprising proteinogenic amino acids

Chan Hu Park, **Sunbum Kwon***

Department of Chemistry, Chung-Ang University, Korea

Lasso peptides possess a distinctive [1]rotaxane topology and belong to a group of ribosomally synthesized and post-translationally modified peptides (RiPPs). They are renowned for their exceptional proteolytic, chemical, and thermal stability, likely owing to their [1]rotaxane structure. Consequently, significant research efforts have been dedicated to synthesizing chemically interlocked peptides. However, the organic synthesis of such molecules involves thermodynamically unfavorable processes, such as the formation of preorganized intermediates. In addition, the limited availability of proteinogenic amino acids makes the synthesis even more challenging. Consequently, previous studies have largely focused on grafting peptide segments onto pre-synthesized interlocked organic molecules. In this presentation, we present our approach to craft a mechanically interlocked peptide [2]rotaxane using only proteinogenic amino acids. The key of this synthetic method lies in forming a linked three-peptide chain that facilitates simultaneous interlocking and cyclization. Deconjugation between the ring and axle, followed by desulfurization, enables a versatile synthetic method for various peptide sequences.



133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **ORGN.P-210**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

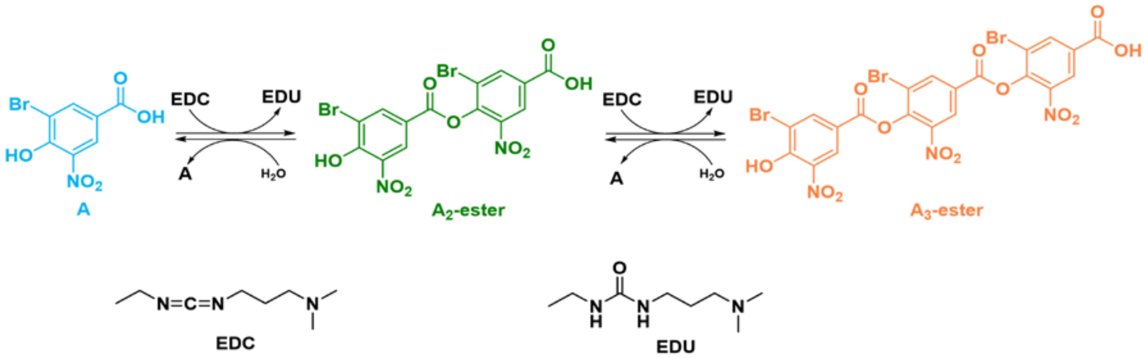
Carbodiimide-fueled dissipative oligoester libraries

Sunbum Kwon[*], **Yeonsoo Lim**[1]

Department of Chemistry, Chung-Ang University, Korea

[1]*Chemistry, Chung-Ang University, Korea*

Major class biopolymers, such as peptides and DNA, are ephemeral. They are synthesized from their monomeric units temporarily activated. On the other hand, their degradation in aqueous environment is spontaneous. These serve as examples of non-equilibrium dissipative systems. Inspired by these natural instances, our group has concentrated on designing the dissipative oligo-esterification of hydroxy acid building blocks. We explored the kinetics of the reversible oligomerization of 3-bromo-4-hydroxy-5-nitrobenzoic acid. The carbodiimide-driven esterification process was meticulously monitored using 1H-NMR spectroscopy, and a numerical fitting of the suggested chemical reaction network to the experimental data was performed. Drawing from this understanding of kinetics, we are currently in the process of constructing an oligo-ester library from multiple building blocks. We anticipate that discovering new non-equilibrium systems controlled by chemical fuels may provide a unique opportunity to mimic functional traits of biopolymers and simulate life-like events in a laboratory setting.



Poster Presentation : **ORGN.P-211**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Evaluation of Polyvinylpyrrolidone as a Dispersant for Ultra-thin Dielectric Sheet with Excellent Chemical and Mechanical Properties

Young-O Kim, Jung Jin Park[1], Jong Ho Lee[1,*]

MLCC Process Architecture Lab, Samsung Electro-Mechanics, Korea
[1]*MLCC Green Chip Lab, Samsung Electro-Mechanics, Korea*

Uniform dispersion of nanoparticles (NPs) in polymeric binders determines the mechanical properties of dielectric sheets (or green sheet), which can reduce some factors generating the electrical failure of multi-layer ceramic capacitor (MLCC). Pertinent selection of dispersants is crucial for optimizing the interfacial interaction between the surface of NPs and binders. General strategies for designing dispersants make chemical structures of dispersants similar to those of binders for increasing material compatibility. However, to diversify the range of material choice, dispersants with the different chemical structure with the binders need to be considered. In this study, we selected polyvinylpyrrolidone (PVP) as a dispersant for dispersing barium titanate (BaTiO3) NPs and incorporated them into a polyvinylbutyral (PVB) binder. We characterized the dispersibility of the BT slurries and the chemical and physical properties of the dielectric composite sheets. It was confirmed that the PVP could be a good candidate as the dispersant for BT NPs to be uniformly dispersed in polymeric binders for producing ultra-thin dielectric sheets with excellent chemical and mechanical properties.

Poster Presentation : **ORGN.P-212**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

NIR fluorescent probes for endogenous CO imaging in bacterial pneumonia

Seokjin Hong, Jusung An, Jaewon Kim, Jungryun Kim, Hyeonji Rha, Eunji Kim, Yujin Kim, Jiyoung Yoo, Changyu Yoon, Jong Seung Kim[*]

Department of Chemistry, Korea University, Korea

Bacterial pneumonia is a respiratory disease that causes several complications which seriously damage human health. Therefore, distinguishing bacterial pneumonia from viral pneumonia is important in pneumonia diagnosis for proper treatment. Our new near-infrared (NIR) probe can selectively diagnose bacterial pneumonia by fluorescence and photoacoustic (PA) dual-mode imaging of endogenous carbon monoxide (CO), a bacterial pneumonia indicator. NO_2-BODIPY reacts quickly and selectively with CO to generate NH_2-BODIPY, which shows excellent NIR fluorescence and PA ability. As a result, NO_2-BODIPY works as an excellent imaging probe with high sensitivity and a clear contrast ratio in cells and bacterial pneumonia mice. To be precise, it can be used as a tissue-penetrating dual imaging probe by producing two-photon excited (1340 nm, σ1 = 1671 GM) NIR fluorescence and PA signals with superior response time and high selectivity, as well as minimized limit of detection (LOD = 20.3 nM). Hence, NO_2-BODIPY has great potential to be applied in precise bacterial pneumonia diagnosis.

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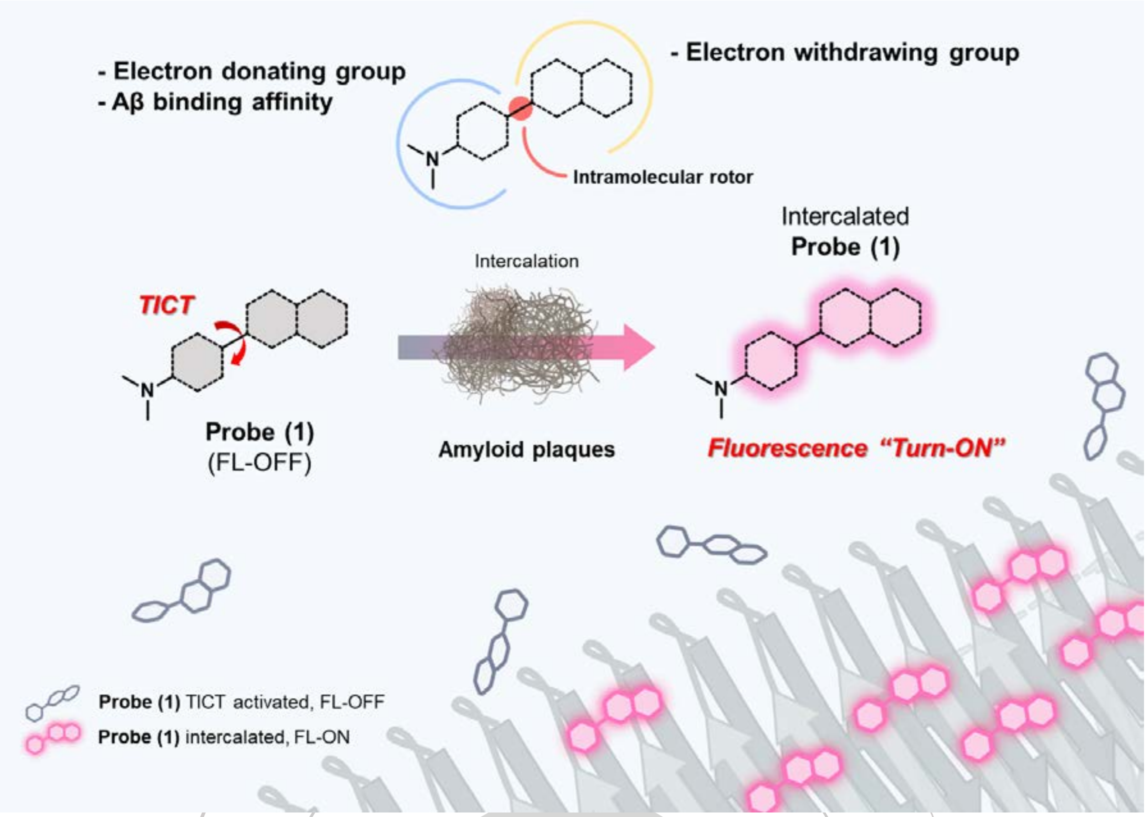
Poster Presentation : **ORGN.P-213**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis and characterization of TICT-based small molecule fluorescent probe for effectual Aβ plaques imaging in Alzheimer's disease brain

Soyu Zi, Jusung An, Jaewon Kim, Jungryun Kim, Hyeonji Rha, Eunji Kim, Changyu Yoon, Yujin Kim, Jiyoung Yoo, Jong Seung Kim[*]

Department of Chemistry, Korea University, Korea

The knowledge and accurate detection of aberrant proteinaceous deposits, such as amyloid-β (Aβ), are pivotal for a comprehensive understanding of Alzheimer's disease (AD) and for developing future diagnostics and clinical intervention strategies. In this study, a novel fluorophore probe (1) was designed based on an electron donor-π-acceptor architecture endowed with a remarkable twisted intramolecular charge transfer (TICT) effect, enabling the clear distinction of the microenvironment of Aβ fibrils. The minimalistic molecule design of probe (1) required only two synthesis steps, making it more economically efficient than universal cross-β-sheet dyes (e.g., Thioflavin T). Probe (1) exhibited excellent selectivity, specificity, and photo-physiological properties toward Aβ fibrils. A binding affinity comparable to ThT was found (Kd = 402.62 ± 236.36 nM), and probe (1) was applied to red-emissive fluorescent staining of amyloid plaques in cortical brain tissue in vitro. As a result, we obtained high-resolution images of amyloid plaques with a remarkable signal-to-noise ratio in transgenic AD-model mice brains. This fluorophore suggests a promising new imaging agent with pragmatic usage and economic advantages.


- Electron donating group
- Aβ binding affinity
- Electron withdrawing group
N
Intramolecular rotor
TICT
N
Probe (1)
(FL-OFF)
Intercalation
Amyloid plaques
Intercalated
Probe (1)
N
Fluorescence "Turn-ON"
Probe (1) TICT activated, FL-OFF
Probe (1) intercalated, FL-ON

Poster Presentation : **ORGN.P-214**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Mechanistic snapshots of rhodium-catalyzed acylnitrene transfer reactions

Hoimin Jung, Sukbok Chang[*]

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

We present a strategic approach to address the long-standing challenge of characterizing the elusive Rh-acylnitrenoid species, which is a highly reactive intermediate that is widely postulated in the C–H amidation catalysis. To address this challenge, we designed a chromophoric octahedral rhodium complex ligated with a bidentate dioxazolone, which can serve as an acylnitrenoid precursor under photochemical reaction conditions. This new rhodium complex serves as an acylamido precursor for photocatalytic hydrocarbon amidation. Through X-ray photo crystallographic analysis of the rhodium-dioxazolone complexes, we successfully captured and characterized the elusive Rh-acylnitrenoid species, providing key mechanistic insights into nitrenoid transfer pathways. We also monitored in crystallo reaction monitoring between postulated Rh-acylnitrenoid species and cocrystallized acetone, which further corroborates the electrophilic reactivity of postulated intermediate.

Poster Presentation : **ORGN.P-215**

Organic Chemistry

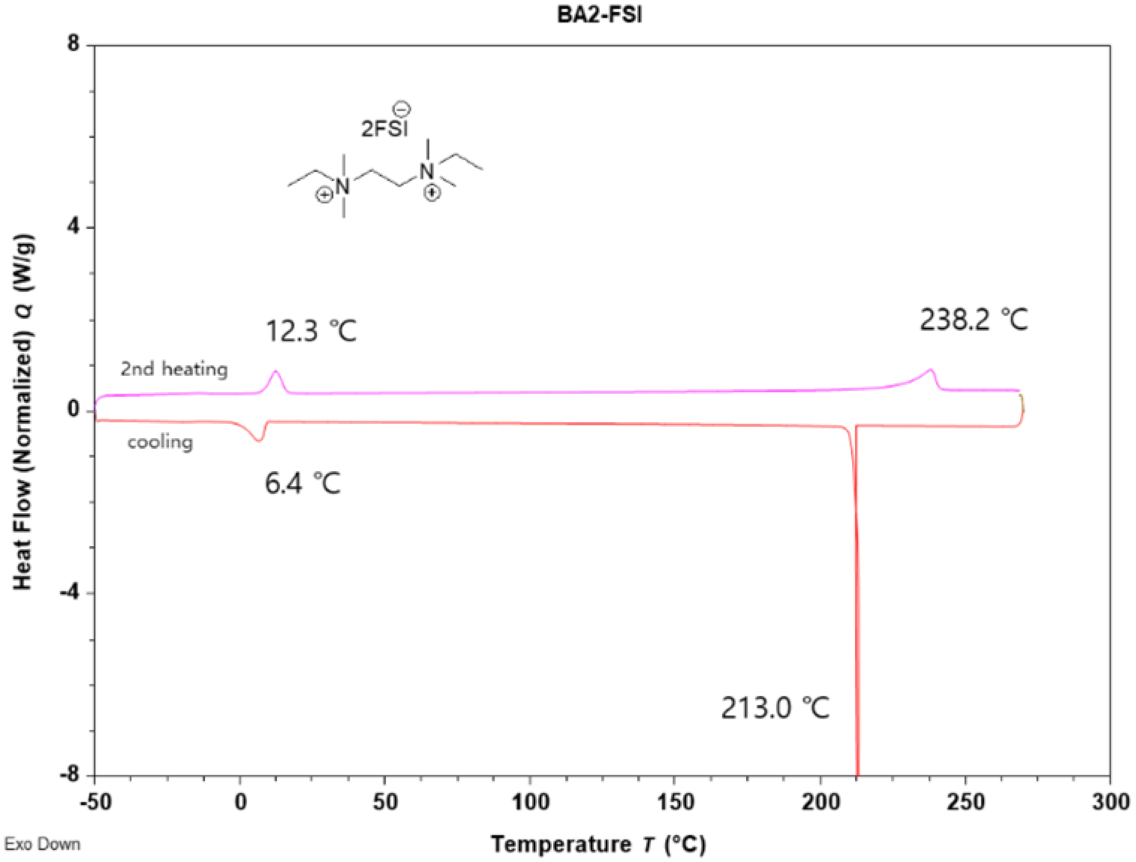
Exhibition Hall 2 FRI 11:00~13:00

Synthesis and characterization of 1,2-bis(*N*-alkyl-*N*,*N*-dimethylammonium)ethane bis(fluorosulfone)imide and bis(trifluoromethanesulfone)imde salts

Giseon Ryu, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

Organic ionic plastic crystals (OIPCs) offer advantages as a solid electrolyte due to their soft solid-state nature, plasticity, non-flammability, and ion conductivity. Our research group has synthesized novel OIPCs by combining various dication structures with Br^-, PF_6^-, Tf_2N^-, and BF_4^- anions. In this study, we applied either bis(fluorosulfone)imide (FSI) or bis(trifluoromethanesulfone)imde (Tf_2N) anions to 1,2-bis(*N*-alkyl-*N*,*N*-dimethylammonium)ethane cations and thoroughly characterized the new compounds. The chemical structures of the new bis-ammonium salts were confirmed by ^1H NMR. Using differential scanning calorimetry (DSC), 1,2-bis(*N*-ethyl-*N*,*N*-dimethylammonium)ethane FSI exhibited one solid-solid phase transition at $T_{ss} = 12$ ℃. This compound showed low entropy of fusion, 32 J $K^{-1}mol^{-1}$, which is low enough to be categorized as a plastic crystal. Detailed characteristics of the synthesized material will be presented in the poster.


BA2-FSI
2FSI
N
N
8
4
0
-4
-8
Heat Flow (Normalized) Q (W/g)
12.3 ℃
238.2 ℃
2nd heating
cooling
6.4 ℃
213.0 ℃
-50
0
50
100
150
200
250
300
Temperature T (°C)
Exo Down

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Poster Presentation : **ORGN.P-216**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

[Withdrawal] Tumor-Activated Prodrug with Synergistic Anti-Stemness Chemical and Photodynamic Therapies

Jaewon Kim, Jusung An, Hyeonji Rha, Eunji Kim, Changyu Yoon, Huiyeon Moon, Yujin Kim, Jiyoung Yoo, Dongeun Kim, Dongeun Kim*

Department of Chemistry, Korea University, Korea

Poster Presentation : **ORGN.P-217**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Combinatorial therapy for enhanced rheumatoid arthritis (RA) treatment based on small molecule

Changyu Yoon, Jusung An, Jungryun Kim, Jaewon Kim, Hyeonji Rha, Eunji Kim, Yujin Kim, Huiyeon Moon, Jiyoung Yoo, Jong Seung Kim[*]

Department of Chemistry, Korea University, Korea

Sonodynamic Therapy (SDT), known for its deep tissue penetration and non-invasive characteristics, presents a novel solution for managing difficult-to-treat lesions. However, there is notable scarcity of small molecule-based therapies in this field, especially for rheumatoid arthritis (RA). Most therapeutic approaches rely on encapsulating treatments within nanoparticles or employing macromolecules for delivery. However, adopting small molecule-based treatments is especially advantageous due to their ease of chemical modification, high reproducibility, and biocompatibility. Based on these advantages, we are developing a unique, combinatorial, and activatable sonosensitizer specifically designed for RA. This compound integrates three essential functional components. It utilizes either methylene blue or porphyrin as the sonosensitizing agent. it includes a responsive group that targets peroxynitrite ($ONOO^-$), which is typically found in excess in arthritic joints, and this responsive group is engineered to release Methotrexate (MTX), a conventional RA treatment drug, upon activation. This targeting mechanism holds the potential for an enhanced therapeutic effect, especially upon further optimization of the metal component. Our design of this combinatorial therapy for RA aims at ensuring predictability and minimizing side effects, a notable advancement over conventional sonosensitizers used in RA treatment. Additionally, it's a strategy that enables dual therapeutic effects through a single, simple small-molecule structure. This research holds immense potential for providing a significant breakthrough in addressing the challenges of rheumatoid arthritis, offering a promising new avenue for treatment.

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Poster Presentation : **ORGN.P-218**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Mechanistic Study of Palladium-Catalyzed Amination of Densely Functionalized Aryl Halides

Suyeon Kim, Seoung-Tae Kim[1], Mu-Hyun Baik[2,*]

Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea
[1]*Department of Chemistry, Massachusetts Institute of Technology, United States*
[2]*Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Coupling reactions become challenging as the complexity of the substrates increases due to a potential inhibition by various functional groups. The Buchwald group proposed a method employing stoichiometric amounts of Pd-complexes for the amination of densely functionalized aryl halides, however, the catalytic variant proved inefficient. Suppose the underlying mechanistic factors for the disparate reactivity between stoichiometric and catalytic conditions were identified. In that case, it might pave the way for the design of effective strategies to overcome these challenging catalytic transformations. Herein, we present a combined theoretical and experimental investigation to achieve catalytic rivaroxaban amination as a representative example. Armed with a plausible mechanism and awareness of potential issues, computational and experimental approaches propose and validate an essential problem-solving strategy involving the reversibility of putative off-cycle species.

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Poster Presentation : **ORGN.P-219**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Complexation-induced Assembly of Imine-linked Aromatic Foldamer Receptors

Geunmoo Song, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

Aromatic foldamers function as synthetic receptors that create the binding cavities through folding process. We synthesized indolocarbazole-naphthyridine oligomers which have internal tubular cavities with hydrogen-bonding donors and acceptors, thereby allowing to bind polyols and carbohydrates. Imines are known to form in-situ from their precursors, aldehydes and amines, yielding solely water as a byproduct. However, imines do not form quantitatively in solution: Instead, they exist in equilibrium mixtures with their precursors due to the dynamic nature of imine bonds. In this study, the imine bond is used to synthesize foldamer receptors, with the hypothesis of complexation-induced equilibrium shifting. We have clearly demonstrated that imine-linked longer foldamers are assembled quantitatively only in the presence of a guest capable of strong binding. Interestingly, the receptors exhibit adaptive folding properties as well as temperature-dependent guest selection. Details including the synthesis, binding properties, and folding structures of these foldamer receptors will be discussed in the presentation.

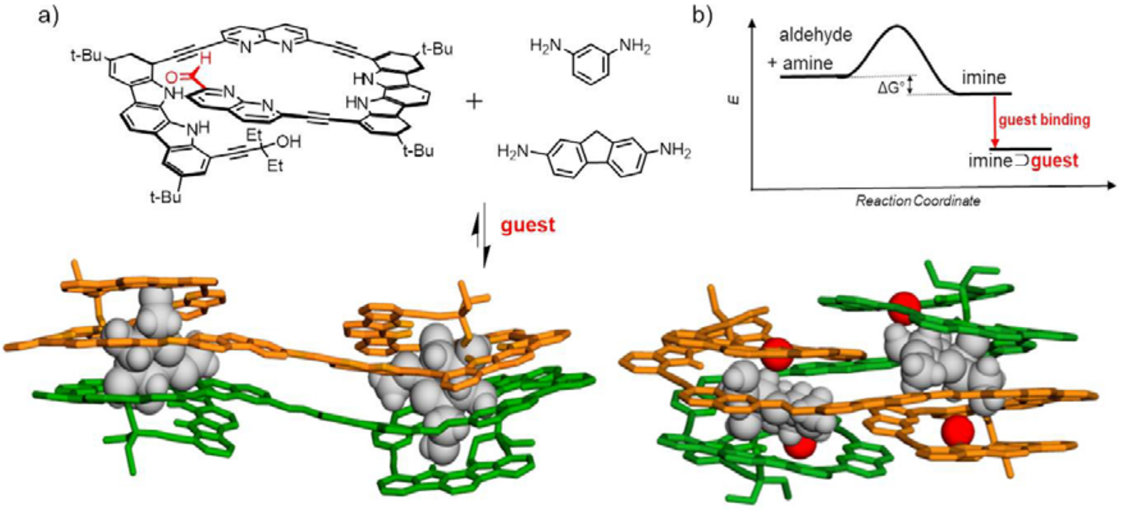

Figure. a) Molecular structures of foldamer with an aldehyde and aromatic diamines (up), and X-ray crystal structures of imine-linked foldamer receptor-guest assemblies (down). b) Hypothetical energy profile for a complexation-equilibrium shift toward imine formation.

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Poster Presentation : **ORGN.P-220**

Organic Chemistry

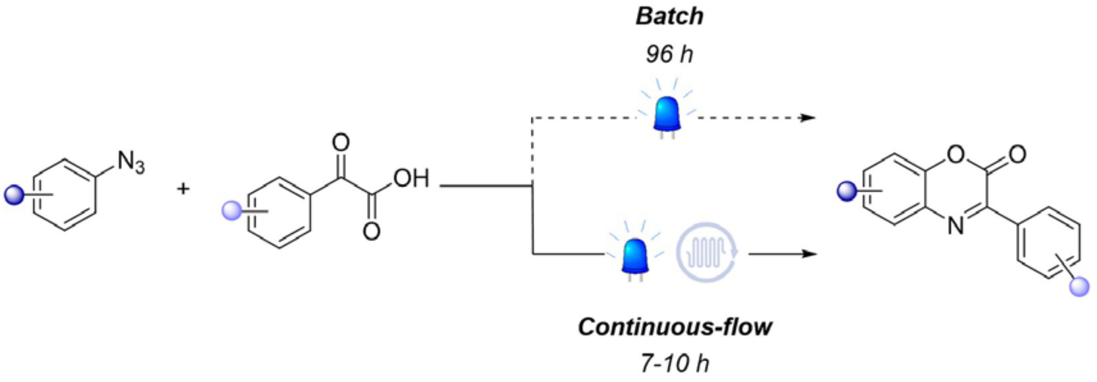
Exhibition Hall 2 FRI 11:00~13:00

Photosensitizer-Free Benzo[1,4]oxazin-2-one Synthesis by Continuous-Flow Photochemistry

Eunhui Park, Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

2H-Benzo[b][1,4]oxazin-2-ones have been widely explored in many applications exhibiting significant biological and pharmaceutical attributes. We propose a photochemical approach for the synthesis of benzo[1,4]oxazin-2-one derivatives from azides and α-arylglyoxylic acids under blue LED irradiations. This study represents the first utilization of azides to access diverse benzo[1,4]oxazin-2-ones. Notably, this process is mild and eco-friendly, not requiring any external additives. Moreover, we have incorporated a continuous-flow system into our methodology, which significantly enhances the efficiency of the batch reaction. This continuous-flow method drastically reduces reaction times, making it a highly advantageous over conventional methodologies.



- *mild condition*
- *eco-friendly*
- *improved efficiency*

Poster Presentation : **ORGN.P-221**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Photoredox/Nickel Dual Catalytic Enantioselective Synthesis of α-Chiral Sulfones Using Sulfonyl Chlorides

Doyoung Kim, Sungwoo Hong*

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

This research delves into the enantioselective hydrosulfonylation of various α,β-unsaturated carbonyl compounds using visible light and redox-active chiral Ni-catalysis. The aim is to facilitate the synthesis of enantioenriched α-chiral sulfones with remarkable enantioselectivity, exceeding 99% ee. A significant challenge involves enhancing the reactivity between chiral metal-coordinated carbonyl compounds and moderate electrophilic sulfonyl radicals, with the goal of minimizing background reactions. The success of the approach relies on two distinctive attributes: 1) the use of Cl-atom abstraction for sulfonyl radical generation from sulfonyl chlorides, and 2) the single-electron reduction to produce a key enolate radical Ni-complex. The latter process appears to enhance the feasibility of the sulfonyl radical's addition to the electron-rich enolate radical. An in-depth investigation into the reaction mechanism, supported by both experimental observations and theoretical analysis, offers insight into the intricate reaction process. Moreover, the versatility of the methodology is highlighted through its successful application in the late-stage functionalization of complex bioactive molecules, demonstrating its practicality as a strategy for producing α-chiral sulfones.

Poster Presentation : **ORGN.P-222**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

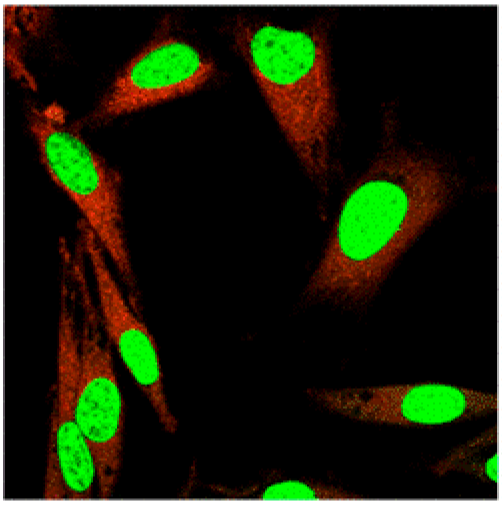
Hydrophilic Heavy-Atom-Free Photosensitizers: NI-Cz for Nucleus-Targeted Fluorescence Bioimaging and Photodynamic Therapy

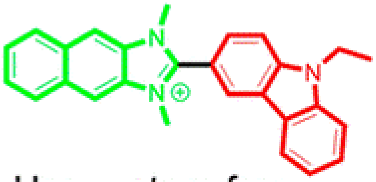
Gahyun Kim, Seongman Lee[1], Songyi Lee[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea

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

Enhancing the process of intersystem crossing (ISC) and the generation of reactive oxygen species (ROS) has traditionally involved the incorporation of heavy atoms into photosensitizers (PSs). However, ongoing concerns about the cost and dark toxicity associated with heavy metals have led to increased interest in designing molecular structures using heavy-atom-free PSs. The photophysical properties of imidazole derivatives have demonstrated robust fluorescence emission and efficient ROS generation. Furthermore, possessing excellent electron-withdrawing capability, integration of electron-donating groups into the imidazolium scaffold can induce a potent intramolecular charge transfer (ICT) effect. This effect leads to a red shift in absorption and emission wavelengths and enhances two-photon absorption (TPA) characteristics, including wavelength (λ_{TPA}) and absorbance (δ_{TPA}). Additionally, imidazolium salts exhibit hydrophilicity, enabling them to maintain fluorescence emission and ROS generation capabilities in aqueous environments while displaying selective antimicrobial activity against Gram-positive bacteria. Therefore, we developed NI-Cz, a heavy-atom-free photosensitizer utilizing naphthoimidazolium as the acceptor. This NI-Cz PS demonstrated outstanding fluorescence emission (Φ_F = 0.22) and ROS generation (Φ_Δ = 0.49), even in highly aqueous environments, and was confirmed through fluorescence bioimaging and photodynamic therapy (PDT) in cancer cells. It exhibited negligible dark toxicity. Furthermore, NI-Cz showed selective nuclear localization and effective PDT therapeutic efficacy against Gram-positive bacteria. Additionally, efficient TPA cross-section and a type I ROS generation mechanism were observed.





- ✓ Heavy-atom-free
- ✓ ROS generation
- ✓ Fluorescence emission
- ✓ Water solubility
- ✓ Nucleus localization
- ✓ Gram-positive bacteria
- ✓ Two-photon absorption

Poster Presentation : **ORGN.P-223**

Organic Chemistry

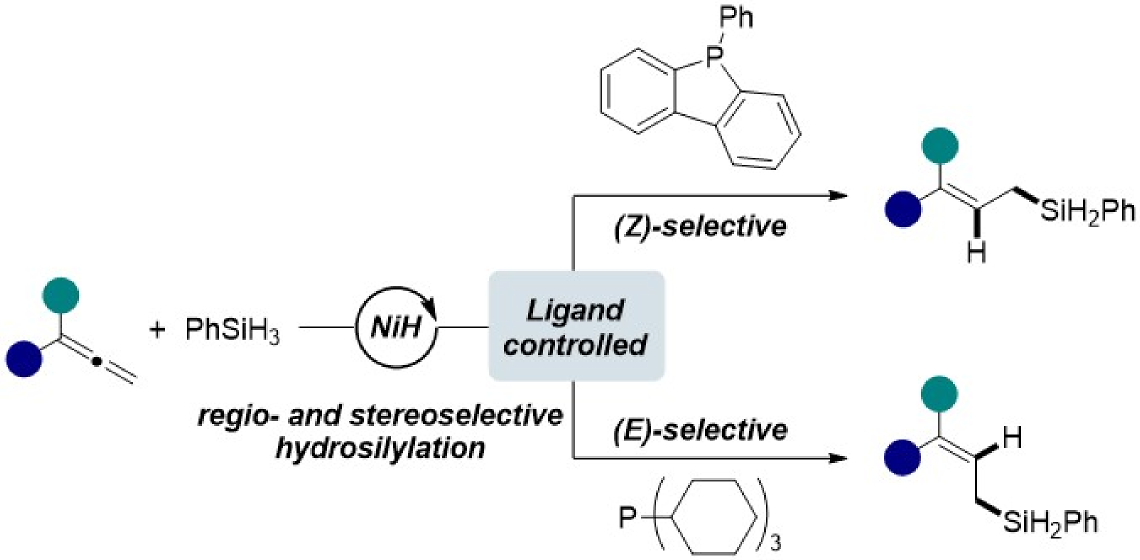
Exhibition Hall 2 FRI 11:00~13:00

Nickel-Catalyzed Stereo-Controlled 2,3-Hydrosilylation of 1,1-Disubstitutedallenes

Jin A Kim, Jihoon Jang, Eun Jin Cho[*]

Department of Chemistry, Chung-Ang University, Korea

Directing regioselectivity and stereoselectivity in reactions of allenes has presented significant challenges, due to the several available options. In this work, we have successfully developed a Ni-catalyzed regio- and stereoselective 2,3-hydrosilylation of terminal allenes. We have manipulated the stereoselectivity by strategically implementing ligand-induced steric effects. The use of phenyl dibenzophosphole resulted in the generation of Z-selective alkenes, whereas the employment of tricyclohexylphosphine (PCy3) yielded E-selective alkenes. This selective control of alkene geometry through ligand choice represents a significant advancement in the field of stereochemistry.



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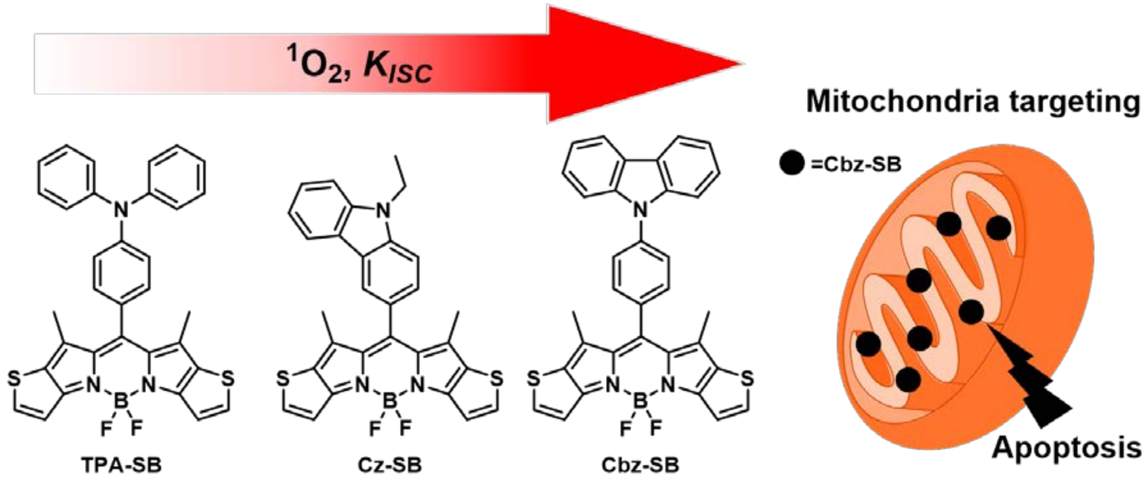
Poster Presentation : **ORGN.P-224**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Thiophene-fused BODIPYs for verification of mitochondrial targeting ability and $^1O_2$ generation

<u>Suhong Min</u>, Songyi Lee[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

The conventional photosensitizers (PSs) used in photodynamic therapy (PDT) have shown potential for cancer treatment. Such PSs necessitate efficient intersystem crossing (ISC) and these existing PSs come with several drawbacks. These drawbacks include potential dark toxicity in non-cancerous tissues, low efficacy under hypoxic conditions, non-specific targeting during treatment, and limited fluorescence imaging capabilities. In this study, the thiophene-fused BODIPY chromophore exhibits significant potential for PDT due to its efficient generation of reactive oxygen species (ROS) in the highly excited triplet state. Thus, we efficiently generated the triplet excited state to achieve heavy-atom-free PSs (Thiophene-fused BODIPYs) with high $^1O_2$ generation efficiency and fluorescence quantum yield. Furthermore, the introduction of sulfur atoms and the extended π-conjugation will lead to a decrease in electron density, thereby enhancing the mitochondrial-targeting capability compared to the non-fused BODIPY core. We synthesized the compound R-SB (TPA-SB, Cz-SB, Cbz-SB) by fusing thiophene onto the BODIPY core to extend π-conjugation and by introducing electron-donating groups at the *meso* position. Among these, Cbz-SB exhibited higher fluorescence quantum yield, $^1O_2$ quantum yield, and mitochondrial targeting capability compared to TPA-SB and Cz-SB. Ultimately, this research can be considered optimized for targeting essential cellular organelles in short working radius PDT processes, and it will aid in the design of future heavy-atom free PSs.



$^1O_2$, K_{ISC}
Mitochondria targeting
● =Cbz-SB
Apoptosis
TPA-SB
Cz-SB
Cbz-SB

Poster Presentation : **ORGN.P-225**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

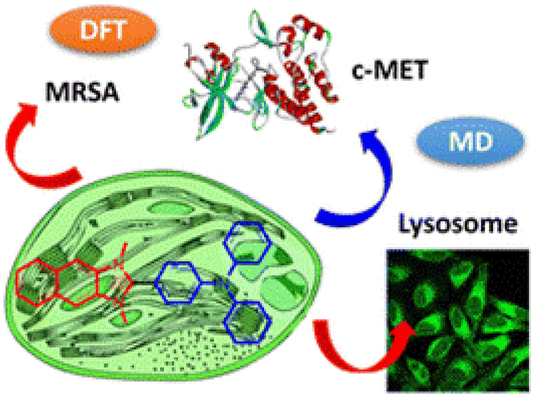
Dual anticancer and antibacterial activity of promising potential fluorescent naphthoimidazolium derivatives.

Minseok Yoo, Seongman Lee[1], Songyi Lee[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea

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

Cancer has emerged as a significant global health challenge, ranking as the second leading cause of death worldwide. Moreover, cancer patients frequently experience compromised immune systems, rendering them susceptible to bacterial infections. Combining anticancer and antibacterial properties in a single drug could lead to improved overall treatment outcomes and patient well-being. In this context, the present study focused on a series of hydrophilic naphthoimidazolium salts with donor groups (NI-R), aiming to create dual-functional agents with antibacterial and anticancer activities. Among these compounds, NI-TPA demonstrated notable antibacterial activity, particularly against drug-resistant bacteria, with MIC value of 7.8 μg/mL. Furthermore, NI-TPA exhibited the most potent cytotoxicity against four different cancer cell lines, with an IC_{50} range of 0.67-2.01 μg/mL. The observed high cytotoxicity of NI-TPA agreed with molecular docking and dynamic simulation studies targeting c-Met kinase protein. Additionally, NI-TPA stood out as the most promising candidate for two-photo excitation, fluorescence bioimaging, and localization in lysosomes. This study presents a novel design of imidazolium salts with promising potential for phototheranostic applications in cancer treatment and bacterial infections.


DFT
MRSA
c-MET
MD
Lysosome

Poster Presentation : **ORGN.P-226**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Selective Synthesis of β-Fluoro-α,β-Unsaturated Amides via Palladium-Catalyzed Aminocarbonylation of 1-Fluoro-2,2-Diiodovinylarenes

Chae Eun Song, Karthik Rajan Rajamanickam, Yubin An, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

A novel synthetic strategy for the selective preparation of (*Z*) and (*E*)-β-fluoro-α,β-unsaturated amides via palladium-catalyzed aminocarbonylation of 1-fluoro-2,2-diiodovinylarenes has been developed and thoroughly investigated. Employing Allylpalladium(II) chloride dimer as the catalyst and DBU as a base in DMF solvent led to the predominant formation of the (*Z*)-isomer. Conversely, utilizing an Xantphos ligand in conjunction with Allylpalladium(II) chloride dimer and Triethylamine as a base in 1,4-dioxane solvent facilitated the selective synthesis of the (E)-isomer. Remarkably, 1-fluoro-2,2-diiodovinylarenes bearing diverse substituents on the phenyl ring underwent reactions with various secondary amines, resulting in the corresponding (*Z*)-isomeric amides with high yields and selectivity. In contrast, the (*E*)-isomeric amides exhibited comparatively lower yields and limited applicability. Our findings provide an efficient synthetic methodology for β-fluoro-α,β-unsaturated amides and underscore the potential of 1-fluoro-2,2-diiodovinylarenes as valuable precursors in palladium-catalyzed carbonylations.

Poster Presentation : **ORGN.P-227**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of a highly sensitive fluorophore to detect amyloid-beta fibrils through dioxaborine-based biannulated π-structure expansion

Dongeun Kim, Jusung An, Jungryun Kim, Hyeonji Rha, Jaewon Kim, Eunji Kim, Changyu Yoon, Yujin Kim, Jiyoung Yoo, Jong Seung Kim[*]

Department of Chemistry, Korea University, Korea

Alzheimer's disease (AD) is the most common neurodegenerative disease, but its pathophysiology is still not fully understood despite extensive research. Amyloid-beta (Aβ) aggregates formed due to protein misfolding are a well-known indicator of AD. To diagnose AD early and understand its complex pathology, it is crucial to visualize Aβ aggregates selectively. A highly hydrophobic property and a dioxaborine-based curcumin structure have been found to have a strong affinity for Aβ fibril. Based on this, two organic small-molecule dioxaborine-derived fluorophores were created by adjusting the hydrophobicity to improve the binding affinity for Aβ1-42 fibrils and prevent low aqueous solubility by using biannulate donor motifs in D-π-A dye. The resulting fluorophore has red emission and a significant stoke shift, and it has been found to have a picomolar high affinity for Aβ fibrils. This is expected to enable more efficient scanning of Aβ fibrils and may serve as the basis for a new imaging agent that can detect AD at an early stage.

Poster Presentation : **ORGN.P-228**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Developing a therapy that specifically targets Triple-Negative Breast Cancer

Yujin Kim, Jusung An, Jungryun Kim, Hyeonji Rha, Jaewon Kim, Jiyoung Yoo, Huiyeon Moon, Changyu Yoon, Yubin Lee[1], Jong Seung Kim*

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

TNBC is a highly heterogeneous disease, and tumors commonly contain cancer stem cell-like populations with increased self-renewal, tumor invasion, and metastatic abilities. We herein present a new small molecule-based dual prodrug, Nic-En, combining a signal transducer and transcriptional activator 3 (STAT3) inhibitor, Niclosamide and Enzyme-triggered cleavage moiety. Nic-En is designed to target triple-negative breast cancer CSCs, specifically activated in the Tumor microenvironment and suppress CSC properties by inhibiting STAT3. Through this strategy, Nic-En can provide therapeutic benefits for treating TNBC.

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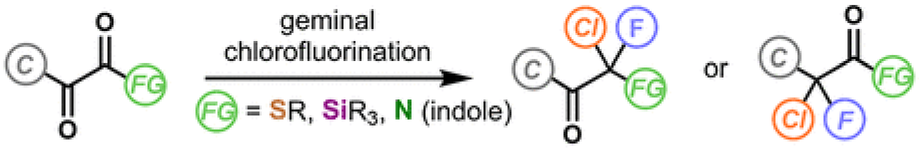
Poster Presentation : **ORGN.P-229**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

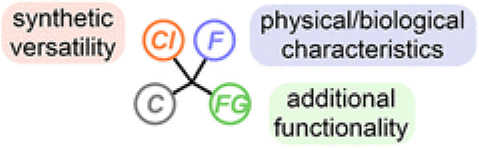
Access to Multifunctionalized Tetrasubstituted Carbon Centers Bearing up to Three Different Heteroatoms via Tandem Geminal Chlorofluorination of 1,2-Dicarbonyl Compounds

Mugeon Song, Won-jin Chung[1,*]

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

The incorporation of noncarbon heteroatoms into organic molecules typically instills characteristic and often valuable functionalities. The copresence of different heteroatoms can further broaden their utility through the synergistic cooperative effects, which may even lead to the discovery of formerly unavailable properties that are not just a simple accumulation of each function. However, despite increasing interest in the controllable installation of heteroatoms, it has been extremely challenging to construct carbon centers having three different heteroatoms in a synthetically useful manner. In this work, our group's tandem geminal chlorofluorination (Cl, F) strategy was applied to rationally designed heteroatom-bearing 1,2-dicarbonyl substrates, including α-keto thioesters (S), α-keto *N*-acylindoles (N), and α-keto acylsilane (Si), which resulted in the practical production of doubly or triply heterofunctionalized tetrasubstituted carbon centers with excellent site-selectivity.





- ♦ densely hetero-functionalized carbon
- ♦ up to three different heteroatoms
- ♦ rational substrate design
- ♦ mild and convenient process


사단법인
대한화학회
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Poster Presentation : **ORGN.P-230**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Computational Study on Metal-Ligand Cooperativity in Dicopper Catalyzed Azide-Alkyne Cycloaddition Reactions

Hyoju Choi, Cody B. van Beek[1], Daniël L. J. Broere[1,*], Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Chemistry, Utrecht University, Netherlands*

Over the past two decades, considerable effort has been devoted to understanding the mechanism of the copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction with various ligands. In this study, we present the synthesis and characterization of neutral dicopper complexes featuring the proton-responsive dinucleating $^{i\mathrm{Pr}}$PNNP ‘expanded pincer’ ligand. Mechanistic studies were conducted through a combination of isotopic labeling experiments and density functional theory (DFT) calculations, focusing on the proton transfer of CuAAC. The investigation reveals that the formation of the triazole product proceeds via a stepwise metal-ligand cooperative (MLC) pathway. This proposed mechanism is favored over the direct alkyne-to-triazolide proton transfer, as it requires less structural reorganization of the dicopper platform. Our findings elucidate how cooperativity between the copper centers and the $^{i\mathrm{Pr}}$PNNP ligand can introduce an alternative mechanistic pathway, circumventing the conventional rate-limiting alkyne-to-triazolide proton transfer. This study deepens our understanding of metal-ligand cooperativity in CuAAC, providing valuable insights for the development of more efficient and sustainable synthetic methodologies.

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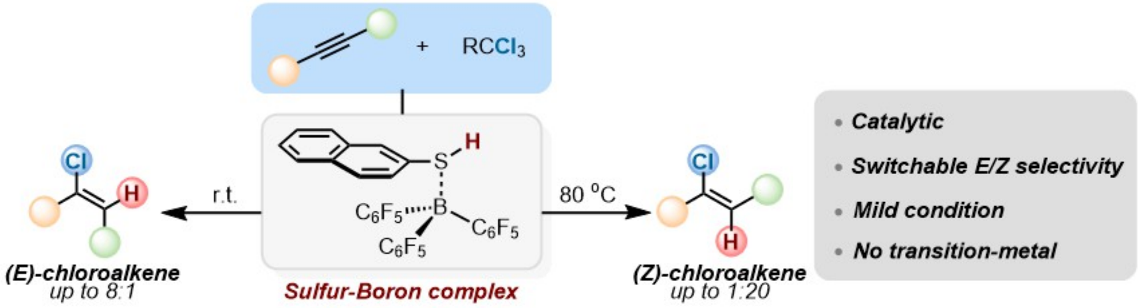
Poster Presentation : **ORGN.P-231**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Lewis Pair-Catalyzed Hydrochlorination of Alkynes to Chloroalkenes with Switchable E/Z Selectivity

Yun Soo Shim, Hyung Min Chi[*]

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

A catalytic, and switchable synthesis of chloroalkenes from alkynes via sulfur-boron Lewis pair complex has been developed. The catalytically active Lewis pair complex were formed with the combination of 2-naphthalenethiol and B(C6F5)3. Both E and Z chloroalkenes were obtained in good yields with high selectivities by simply controlling the reaction temperature. Thorough mechanistic studies revealed that hydrochlorination proceeds through the hydrogen atom transfer between the sulfur-boron complex and the alkyne substrate by forming reactive vinyl radical species, followed by capturing in situ generated chlorine radicals. This work provides new opportunities for selective synthesis of chloroalkenes using the main group catalysts.



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Poster Presentation : **ORGN.P-232**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Visible-Light-Driven Sulfonamidation via One-Pot Multicomponent Reaction of Arylazo Sulfones, DABSO, and Amines

Truong Giang Luu, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Sulfonamide structures are of great importance in organic chemistry because they are frequently found in many molecules including natural products and pharmaceuticals. As a result, various manufacturing techniques for sulfonamides have been developed over several decades. Recent advancements in organic reactions utilizing visible light as an energy source have contributed to organic chemistry field. In this study, we present a visible-light-promoted approach for synthesis of sulfonamides from arylazo sulfones. One-pot tri-component reactions were performed by combinding arylazo sulfones, DABSO, and amines and using $CuBr_2$ as a coupling catalyst. The reaction was carried out by irradiation with blue LEDs, resulting in the preparation of various sulfonamides in good yields under mild conditions. This method has proven effective for generating a variety of sulfonamides relevant for pharmaceutical applications.

Poster Presentation : **ORGN.P-233**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Tin (II) Chloride-Mediated Reaction for the Transformation of *tert*-Butyl Esters to Carboxylic Anhydrides

Anh Thu Nguyen, Hee-Kwon Kim[*]

Department of Nuclear Medicine, Jeonbuk National University, Korea

Anhydrides are important functional groups in chemistry and have been widely employed in industry to produce a wide range of products such as pharmaceuticals, food additives, dyes and resins. In organic synthesis, anhydrides are commonly used as acylating agents and substrates or intermediates in various transformations. Anhydrides are commonly prepared from highly reactive acyl halides or from carboxylic acids. *tert*-Butyl groups have been widely used to protect esters because they prevent the formation of unwanted side products while carrying reaction. Herein, we present the synthesis of anhydrides via a one-pot reaction employing *tert*-butyl esters, α,α-dichlorodiphenylmethane and carboxylic acids as substrates and tin (II) chloride as a catalyst. Several symmetrical and asymmetrical anhydrides were successfully prepared within two hours under room temperature, providing a facile and efficient synthetic methods to afford anhydrides.

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Poster Presentation : **ORGN.P-234**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Visible-Light-Driven Copper-Catalyzed Reaction of Aldehydes with O-Benzoyl Hydroxylamines for the Formation of Amides

Anh Thu Nguyen, Hee-Kwon Kim[*]

Department of Nuclear Medicine, Jeonbuk National University, Korea

Amides are one of the most important functional groups in organic chemistry and amide moieties are present in the structures of various pharmaceuticals, bioactive compounds, and biomolecules. In organic synthesis, amides have been used as useful starting materials for producing a wide range of compounds, for instance, azides, ureas, heterocycles, alkynes, and ketones. Therefore, it is crucial to develop efficient amide bond formation reactions. Photoreactions are the types of transformation that use visible light as source of energy to initiate the reactions. In this study, we present a synthetic method of amides from aldehydes, benzoyl hydroxylamines and *tert*-butyl hydroperoxide via a visible-light-mediated reaction catalyzed by copper. A variety of aliphatic and aromatic aldehydes and benzoyl hydroxylamines were successfully transformed into the desired amides in good yields. providing an effective method to synthesize amides under mild conditions.

Poster Presentation : **ORGN.P-235**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Rhodium-catalyzed Regiodivergent Double Hydroboration of Pyridine

Seung Hyun Lee, Hyoju Choi, Sehoon Park[1,*], Mu-Hyun Baik[*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]*Chemistry, Guangdong Technion Israel Institute of Technology, China*

Dihydropyridine(DHP) is one of ubiquitous motifs found in natural products and widely used in medicinal chemistry. To tailor its properties for specific applications, chemists have developed several approaches to synthesize functionalized DHP. The hydroboration of pyridine is considered one of the most efficient methods for functionalizing DHP, as it provides a synthon that can be readily modified with a high degree of tolerance. The Park group has recently developed the Rh-catalyzed hydroboration of N-heteroarenes, resulting in the double hydroboration of pyridine.1 Despite their success in asymmetric and site-selective double hydroboration of pyridine, the origin of regioselectivity between C3 and C4 positions remains unexplored. Based on density functional theory calculations, we elucidated the detailed mechanism of the double-hydroboration and explained the origin of the observed regioselectivity. By combining the experimental and computational investigations, we proposed that by modulating phosphine ligands, distinct active catalysts can be tailored to control the regioselectivity, which suggested that the active catalyst is a critical determinant of the regioselectivity.

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Poster Presentation : **ORGN.P-236**

Organic Chemistry

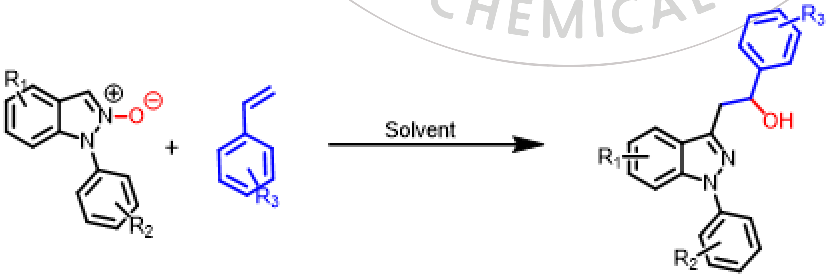
Exhibition Hall 2 FRI 11:00~13:00

Catalyst-Free Synthesis of C3-alkylated 1H-indazoles through Intermolecular [3+2] Cycloadditions.

Jin Kyoon Park[*], **Yong Ju Jang**

Department of Chemistry, Pusan National University, Korea

The direct alkylation of indazoles is one of the most efficient methods to derivatize these molecules for medicinal chemistry studies. Methods for direct C3-functionalization of indazoles are relatively rare, compared to reactions developed for the more nucleophilic N1 and N2 positions. There is not known methods for direct C3-alkylation in catalyst-free conditions before. We was inspired by our previous results, we realized the synthesis of 1H-indazole N-oxides and exploited the multiple C-H functionalization for synthesis of C3-functionalized 1H-indazoles. Herein, we report catalyst-free synthesis of C3-alkylated 1H-indazoles under neat conditions or only by using solvent through intermolecular [3+2] cycloaddition resulted in moderate to good yields.



Poster Presentation : **ORGN.P-237**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Turn-on Detection of Glucose among in aqueous solution at physiological pH using fluorescent probe based on di and tri-peptides with Aggregation Induced Emission characteristic

Inae Jeon, Keun Hyeung Lee[1,*]

Chemistry, Inha University, Korea

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

D-Glucose (Glu) serves as a crucial energy source for vital human organs. In our study, we developed a fluorescent sensor (1) based on monoboronic acid for highly selective ratiometric detection of Glu among various hexoses in aqueous solutions at physiological pH. While the reported sensor (1) exhibited impressive selectivity and sensitivity towards Glu, its practical application in fluorescent cell imaging studies was hindered by drawbacks such as reliance on UV light excitation and emitting at short wavelengths (470 nm). To address this challenge, we introduced a cyano group into the pyrene fluorophore. This strategic modification was aimed at extending both excitation and emission wavelengths, enhancing the Stokes shift values, and emission intensity by constraining intermolecular rotation. The incorporation of the cyano group into the pyrene fluorophore alters its electronic properties, resulting in a shift towards longer wavelengths for excitation and emission. As expected, this new probe (2) has an absorbance wavelength of 420 nm and an emission wavelength in the longer range, i.e., 590 nm. This probe can be applied for cell image study by minimizing interference from background signals.

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Poster Presentation : **ORGN.P-238**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthetic Strategy for ortho-3-propanoate substituted arylphosphonates by a Three Component Coupling Reaction Involving Arynes, Phosphites, and acrylates

Donghwa Shin

chemistry, Sogang University, Korea

A mild and efficient synthetic strategy for the synthesis of ortho-3-propanoate substituted arylphosphonates was developed by a three-component conjugate addition with arynes, phosphites and acylates. Various functional groups were tolerated in the reaction condition, affording diverse ortho-3-propanoate substituted arylphosphonates in moderate to good yields. In addition, the effectiveness of ortho-3-propanoate substituted arylphosphonates obtained under our reaction conditions was investigated. Therefore, the reaction could be utilized for synthesizing a range of organophosphorus compounds found in the natural products, materials, and biologically active compounds.

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Poster Presentation : **ORGN.P-239**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

A new approach for synthesis of amides via C-C bond cleavage

Sueun Lee, Hee Nam Lim[1,*]

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

We report a new method for the synthesis of amides from ketones. The developed method uses activated ketones to synthesize amides using TCFH as a coupling reagent and NMI as a base. It is a one-pot reaction and has the advantage of being able to synthesize amides with good yields under mild reaction conditions. This method features ring opening amidation.

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Poster Presentation : **ORGN.P-240**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

C-C bond cleavage for the synthesis of isocyanates and their applicaion in the preparation of unsymmetrical carbonyl compounds

Seo Yeon Kim, Hee Nam Lim[1,*]

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

Despite considerable progress in the synthesis of unsymmetric carbonyl compounds using different carbonylation reagents, the establishment of dependable and eco-friendly synthetic procedures remains a challenge. In our research, we have identified methyl pyruvate oxime as a viable and safe source of carbonyl, facilitating the synthesis of a wide range of carbonyl compounds via isocyanates as key intermediates. Our investigation primarily targets nitrogen-containing carbonyl compounds, crucial constituents in pharmaceuticals, pesticides, and various functional materials. Through mild one-pot conditions, we have achieved the efficient production of diverse unsymmetrical carbonyl compounds.

Poster Presentation : **ORGN.P-241**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Treat glioblastoma with a temozolomide analog conjugated to lomeguatrib to overcome MGMT resistance

Huiyeon Moon, Jusung An, Jungryun Kim, Hyeonji Rha, Eunji Kim, Changyu Yoon, Yujin Kim, Jiyoung Yoo, Yubin Lee[1], Jong Seung Kim*

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

Glioblastoma, also known as a grade IV astrocytoma, is the most common and dangerous malignant brain tumor in adults. Complete surgical resection is the initial stage in treatment according to the Stupp protocol, which is then followed by concomitant radiotherapy, chemotherapy, and adjuvant chemotherapy. The conventional chemotherapy medication, temozolomide (TMZ), is administered because it may pass through the blood-brain barrier (BBB) and is eaten. The methyl group is transferred by TMZ to the N-7 and O-6 sites of guanine and the O-3 position of adenine in the DNA structure. Guanine methylation at the O-6 position, which results in cell death, is the most dangerous type. MGMT overexpression is believed to be the cause of at least 50% of GBM patients' failure to respond to TMZ, despite the fact that it provides GBM patients some hope. The DNA repair enzyme MGMT removes the alkyl group from O6-methylguanine (O6-MeG). MGMT inhibitors like lomeguatrib, a pseudosubstrate for MGMT, are essential anticancer therapies in order to overcome TMZ resistance.For the tretment of glioblstoma, a small molecule lomeguatrib-conjugated TMZ analog deravitives is synthesized , simulaneously overcoming TMZ resistanace and providing therpeutic benefits

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Poster Presentation : **ORGN.P-242**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

[3 + 2] cycloaddition of nitrile imine with N-silyl enamine from hydrosilylation: Synthesis of pyrazoline derivative

Sooyeon Yun, Seewon Joung[1,*]

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

Pyrazoline, a 5-membered ring heterocyclic compound containing two nitrogen atoms, is pivotal due to its diverse bioactivities. Drugs containing the pyrazoline moiety are used as anticancer drugs, anti-inflammatory drugs, anti-malaria, etc. Our previous studies have focused on the synthesis of cyclic amidines using organic azides with enamine intermediates from the borane-catalyzed hydrosilylation of N-heteroarenes. Enamines showing a variety of applicability for organic synthesis as good nucleophiles, and can be utilized for synthesis of amines, amidines, and other nitrogen containing functional group, showing various application to pharmaceutical chemistry. This study is about construction of pyrazoline ring by using [3 + 2] cycloaddition of the nitrile imine with the N-silyl enamine from the readily available N-heteroarenes.

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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Tailored Covalent Organic Framework with Carbon Nanoparticles for High Efficiency Organic Dye Removal and Solar Distillation of Volatile Organic Compounds

Dhita Azzahra Pancorowati, **Chiyoung Park**[1,*]

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

[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Covalent organic frameworks (COFs) are a type of porous crystalline material that emerges with highly ordered and tunable structures with designer properties. With intrinsic properties like high surface area, adjustable pore size, abundant functional sites, and chemically stable. COFs have been proposed as promising materials for pollutant removal. To cut down the synthesize costs we succeeded in tailoring COFs with carbon nanoparticles (CNPs). This hybrid COF and CNPs (CCNPs) enhance the performance in water pollutant removal, CCNPs can achieve ~99.9% of dye removal within 10 s. Furthermore, introducing CNPs in the system exhibits photothermal effect which can harvest a broad range of wavelengths to be applied for solar distillation process in removal of volatile organic compounds (VOCs) via solar-driven evaporation process. CCNPs exhibits high VOCs rejection of 99.9% under 1 sun irradiation (1 kW m-2). This work provides an effective strategy for rapid organic dye removal and high VOCs rejection via solar-driven evaporation process.

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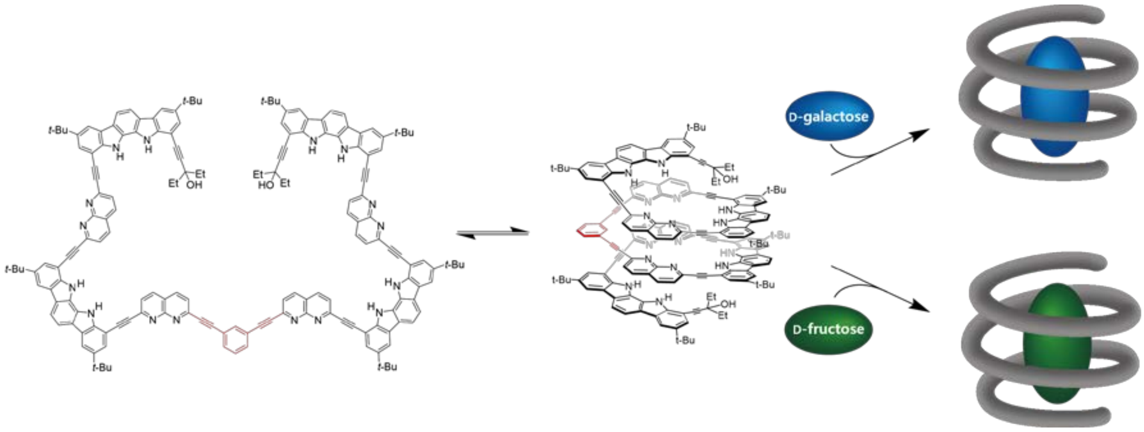
Aromatic Foldamer Receptors Capable of Selectively Binding Monosaccharides

Siwon Yu, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

Aromatic foldamers can adopt folded structures with internal cavities, allowing for binding complementary guest molecules. Recently, we synthesized indolocarbazole-naphthyridine (IN) foldamers[1] in which two repeating monomers were linked through ethynyl bonds. The IN foldamer was proven to bind D-glucose and D-galactose but not D-mannose, forming multiple hydrogen bonds. In this study, we modified the middle of the sequence to alter the shape and dimension of the binding cavity, thus displaying the guest-binding selectivity different from that of the IN foldamers. Indeed, this modified foldamer exhibits selective binding of α-D-galactofuranose among the five structural isomers of D-galactose. More interestingly, the binding energy leads to complete conversion of all D-galactose isomers into α-D-galactofuranose in solution, as confirmed by NMR and Circular Dichroism (CD) spectroscopy analyses. Further details on synthetic procedures and structural analyses will be presented in the poster.References1. Hwang, J. Y.; Jeon, H.-G.; Choi, Y. R.; Kim, J.; Kang, P.; Lee, S.; Jeong, K.-S. *Org. Lett.* **2017**, *19*, 5625.


t-Bu
N
H
HN
Et
OH
HO
D-galactose
D-fructose

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Poster Presentation : **ORGN.P-245**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of oxygen-18-labeled esters from amides using nickel catalysis

Heeju Lee, Nithin Pootheri, Min Woo Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

In this article, we present a novel approach for the synthesis of ^{18}O-labeled esters employing a nickel-catalyzed three-component reaction involving amides, alkyl halides, and ^{18}O-labeled water. This method has been demonstrated to exhibit outstanding selectivity and compatibility across a spectrum of amides and alkyl halides, thereby enabling the synthesis of a diverse array of isotopically labeled esters. The process involves the nickel-catalyzed reaction of alkyl bromides with carboxylates generated from amides and water in the presence of a base, culminating in the efficient formation of the desired esters. This innovative approach holds promise for the facile and selective preparation of isotopically labeled esters with potential applications in various fields of research and industry.

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Poster Presentation : **ORGN.P-246**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Pd-Catalyzed Perdeuteration of Carboxylic Acids

Soo Eun Park, Jung Min Joo[1,*]

chemistry, Kyung Hee University, Korea
[1] *Department of Chemistry, Kyung Hee University, Korea*

Carboxylic acids are prominent building blocks for synthesizing bioactive compounds and functional materials. In the development of carboxylic acid-based materials, the corresponding deuterated compounds are essential for investigating drug metabolism and reaction mechanisms and enhancing stability. We have developed carboxylic acid-directed perdeuteration of arenes. By controlling the steric and electronic properties of ligands, perdeuteration with various arenes could be achieved, even at challenging sp^3 C−H bonds. Strategies to further increase efficiency and expand the scope will also be described.

Poster Presentation : **ORGN.P-247**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Ligand-Enabled Palladium-Catalyzed C-H Alkenylation of Benzoheterodiazoles

Siyeon Jeong, Jung Min Joo[*]

Department of Chemistry, Kyung Hee University, Korea

Pd-catalyzed C-H alkenylation of benzoheterodiazoles containing sulfur, oxygen, and nitrogen has been successfully developed. A careful choice of ligand, solvent, and oxidant enabled high selectivity in the alkenylation with various alkenes. A variety of mechanistic studies including initial rates and DFT computational analysis were conducted. It was observed that our ligand effectively lowered the activation energy of the C-H bond cleavage step. Furthermore, the resulting alkenylated product can be used for the synthesis of phenazine derivatives through a skeletal-editing transformation.

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Poster Presentation : **ORGN.P-248**

Organic Chemistry

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Synthesis and electroluminescent properties of (10-phenylanthracen-9-yl)-indeno-pyridine derivatives for Blue Organic Light-Emitting Diodes

Dong gun Lee, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

The development of efficient blue emitters for organic light-emitting diodes (OLEDs) in the full-color display industry is an important issue. Herein, blue fluorescence materials based on (10-phenylanthracen-9-yl)-indeno-pyridine substituted anthracene derivatives were synthesized and characterized for the efficient blue OLEDs. Their photophysical properties have been investigated. To study their electroluminescent properties, OLED devices were fabricated as following sequence: indium-tin-oxide (ITO) (180 nm) / N,N'-diphenyl-N,N'-(2-napthyl)-(1,1'-phenyl)-4,4'-diamine (NPB) (50 nm) / Blue emitters (30 nm) / bathophenanthroline (Bphen) (30 nm) / lithium quinolate (Liq) (2 nm) / Aluminium (Al) (100 nm). In particularly, a fabricated device using 9,9-dimethyl-7-(10-phenylanthracen-9-yl)-9H-indeno[2,1-b]pyridine as an emitter exhibited efficient blue emission with the luminous efficiency (LE), power efficiency (PE), and external quantum efficiency (EQE) of 0.94 cd/A, 0.67 lm/W, and 1.23 % at 20 mA/cm-2, respectively, and the CIE coordinates of (0.15, 0.09) at 6.0 V.

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Poster Presentation : **ORGN.P-249**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Investigating the influence of substituents on reaction rate in fluorescent probes for mercury and methylmercury detection utilizing displacement reaction of boronic acid with mercury species.

Sumita Subedi, Keun Hyeung Lee[1,*]

Department of chemistry and chemical engineering, Inha University, Korea

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

Our previous chemodosimeter, designated as (a) and incorporating a phenylboronic acid as the reactive site, exhibited selective and sensitive ratiometric signal behavior towards low concentrations of Hg2+ ions in aqueous solutions however reaction rate was slow. To enhance the reaction rate and gain insights into the substituent effect on the reaction rate, we synthesized four fluorescent probe analogs (1-4) containing substituted phenylboronic acids. We investigated their fluorescent response, reactivity, and selectivity towards Hg2+ and CH3Hg+. Introducing an electron-donating methoxy group at the 2nd position of the phenylboronic acid in probe 1 increased the reaction rate for both Hg2+ and CH3Hg+, whereas incorporating an electron-withdrawing fluorine group decreased reactivity. The reaction was completed within 5 minutes for Hg2+ and 15 minutes for CH3Hg+ for probe 1 whereas for probe 4 reaction time was 4 hours for Hg2+ and 5 hours for CH3Hg+. Among these analogs, probe 1 demonstrated the most promising performance for sensing both mercury and methylmercury due to its high solubility, rapid response, ratiometric signal, superior selectivity, and sensitivity. The fluorescence signal of mercury was minimally affected by the presence of other metal ions. The detection limit for Hg2+ was determined to be 4.56 nM based on the linear ratiometric signal response within the nanomolar concentration range of 0–500 nM of mercury ions. Mechanistic studies revealed that probe 1 reacted with Hg2+ to form a covalent product via a replacement reaction of the boronic group, leading to observable fluorescent spectrum changes. Furthermore, we immobilized probe 1 onto TG resin and investigated its application for the removal of Hg2+ and CH3Hg+ from real water samples.

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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Visible Light-Driven Iron-Catalyzed Dual Decarboxylative Csp^3-Csp Cross Couplings

<u>Chaeeun Hong</u>, Yejin Koo, Seokin Han, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

In recent decades, significant attention has been devoted to the study of decarboxylative cross-coupling reactions, driven by the abundance, commercial availability, stability, and ease of handling of organic molecules containing carboxylic acid groups. These reactions have demonstrated the ability of aliphatic, aromatic, and vinyl carboxylic acids to couple with various counterparts in the presence of transition metal catalysts, yielding the desired decarboxylative coupling products in favorable yields. However, the use of alkylating agents as coupling partners in decarboxylative reactions of alkynyl carboxylic acids has been relatively limited. While Mai, Sun, and colleagues reported a copper/silver-catalyzed double decarboxylative coupling reaction involving phenylpropiolic acid and aliphatic acids, this method necessitated high reaction temperatures and was limited to just a few examples. Hence, there is a pressing need for the development of a more versatile method for alkylating alkynyl carboxylic acids in decarboxylative coupling reactions. Herein, we present the iron-catalyzed double decarboxylative coupling reactions between alkynoic acids and alkyl carboxylic acids under photochemical conditions.

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Poster Presentation : **ORGN.P-251**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Electrochemical Synthesis for the Selective Trasformation of Sulfonylhydrazides into Sulfinic and Sulfonic Esters

Yeseul Park, Robin Prakash Sirvin Rajan, Heewon Lee, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Sulfur oxide groups play a vital role in the creation of synthetic intermediates and are commonly present in modified organic materials natural substances, and biologically active compounds like pharmaceuticals and agrochemicals. Through an optimized electrochemical process, sulfinic and sulfonic esters, essential for synthesizing bioactive organic compounds, were selectively derived from arylsulfonyl hydrazides. Extensive exploration of various reaction parameters, including electrolyte, current, and solvent, was conducted to enhance the process. Particularly, the use of MeOH as the solvent resulted in the production of sulfonic esters.

Poster Presentation : **ORGN.P-252**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis of Carbamoyl Fluorides via Visible-Light-Induced Photoredox Organocatalysis Using CF_3SO_2Na and Oxygen

Seonga Jang , **Sun-Joon Min[1,*], KangJoo Lee[2], Do Hoon Cha[2]**

Hanyang University, Korea
[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*
[2]*Department of Applied chemistry, Hanyang University, Korea*

Carbamoyl fluoride (R_2NCOF) is an underexplored functional moiety within the field of organofluoride chemistry, exhibiting substantial potential for diverse biological applications. Originally employed in medicinal chemistry as a precursor for carbamates characterized by exceptional stability and chemical reactivity, this functional group has not been studied comprehensively, primarily due to the paucity of effective synthetic methodologies. Therefore, there is still a need to develop more practical and efficient processes for the synthesis of carbamoyl fluoride.In this presentation, we describe the synthesis of carbamoyl fluoride via visible light-induced DDQ oxidation. This process provides a new method for the facile synthesis of carbamoyl fluoride from secondary amines using sodium trifluorosulfinate, the so-called Langlois reagent, and molecular oxygen. The mechanism is involved in in situ generation of transient carbonyl difluorides (COF_2), which react with amines to form the corresponding carbamoyl fluorides. In addition, the carbamoyl fluorides are readily converted to synthetically useful carbonyl compounds such as ureas, carbamates, and amides under mild reaction conditions. This new synthetic method will provide a simple, metal-free synthetic protocol for valuable carbamoyl fluorides and a new approach to the synthesis of fluorinated materials.

Poster Presentation : **ORGN.P-253**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of a Rhodol based Two-photon Fluorescent Dye for High-resolution in vivo imaging

Min Cheol Park

energy system, Ajou University, Korea

Two-photon (TP) fluorescent dyes with optimal photophysical properties are invaluable for bioimaging, yet they remain scarce. Here, we introduce a novel class of red emissive dyes derived from modifying the rhodol scaffold with fused tetrahydroquinoxaline rings. These dyes exhibit exceptional brightness, high fluorescence quantum yields, and superior two-photon action cross-sections in aqueous solutions, rendering them ideal for deep tissue imaging applications. Moreover, the incorporation of an NHS ester moiety onto the fluorescence probe facilitates straightforward conjugation to Epidermal Growth Factor (EGF), allowing for the exploration of protein-mediated endocytosis pathways.1 Utilizing two-photon microscopy imaging with EGF-conjugated dye, we achieve real-time visualization of receptor-mediated endocytosis dynamics. These dyes hold promise as versatile fluorophore scaffolds for the development of innovative two-photon NIR probes tailored for advanced bioimaging applications.

Development of a Rhodol based Two-photon Fluorescent Dye for High-resolution in vivo imaging.

Min Cheol Park[a] and Hwan Myung Kim [a,*]

[a] *Department of Energy Systems Research and Department of Chemistry, Ajou University, Suwon*
16499, South Korea
Email: kimhm@ajou.ac.kr

Two-photon (TP) fluorescent dyes with optimal photophysical properties are invaluable for bioimaging, yet they remain scarce. Here, we introduce a novel class of red emissive dyes derived from modifying the rhodol scaffold with fused tetrahydroquinoxaline rings. These dyes exhibit exceptional brightness, high fluorescence quantum yields, and superior two-photon action cross-sections in aqueous solutions, rendering them ideal for deep tissue imaging applications. Moreover, the incorporation of an NHS ester moiety onto the fluorescence probe facilitates straightforward conjugation to Epidermal Growth Factor (EGF), allowing for the exploration of protein-mediated endocytosis pathways.[1] Utilizing two-photon microscopy imaging with EGF-conjugated dye, we achieve real-time visualization of receptor-mediated endocytosis dynamics. These dyes hold promise as versatile fluorophore scaffolds for the development of innovative two-photon NIR probes tailored for advanced bioimaging applications.

References

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Poster Presentation : **ORGN.P-254**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Small molecule based two photon photosensitizers: cell organelle targeting strategy

Jong Kyu Baek

energy system, Ajou University, Korea

Research in bioimaging analysis has seen a growing interest in two-photon probes due to their advantages over single photon probes, which can potentially damage live samples due to their high energy and limited tissue penetration. Two-photon probes, utilizing near-infrared light for excitation, offer deeper tissue penetration and minimal phototoxicity. Moreover, they hold promise for photodynamic therapy (PDT). Two-photon photosensitizers (TP-PSs) activate upon near-infrared light exposure, leading to the production of reactive oxygen species (ROS) at targeted regions, thereby inducing cytotoxicity. In this study, we present small-molecule, two-photon activatable dyes tailored for PDT. These dyes feature cell-organelle targeting moieties for precise staining within live cells. TP-PSs demonstrate selective loading into specific organelles such as the endoplasmic reticulum (ER) and Golgi, accompanied by high ROS generation capability. We investigated the PDT efficacy of each PS individually and explored the synergistic effects of their combination

Small molecule based two photon photosensitizers: cell organelle targeting strategy

Min Cheol Park[a], Jong Kyu Baek[a] and Hwan Myung Kim [a,*]

[a] *Department of Energy Systems Research and Department of Chemistry, Ajou University, Suwon 16499, South Korea*
Email: kimhm@ajou.ac.kr

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References

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2. Lee, D. J.; Juvekar, V.; Lee, H. W.; Kim, E. S.; Noh, C. K.; Shin, S. J.; Kim, H. M., *Anal.Chem*. **2021**, *93*, 16821-16827.

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Poster Presentation : **ORGN.P-255**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Enhancing photocatalytic activity in living cells with Metal Modulation

Yubin Lee, Jusung An, Jungryun Kim, Hyeonji Rha, Jaewon Kim, Eunji Kim, Changyu Yoon, Yujin Kim, Huiyeon Moon, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Photoredox catalytic chemistries have had a remarkable impact on the field of anticancer therapy, enabling the regulation of biochemical processes. Nevertheless, developing novel photoredox catalysts for living systems or enhancing the catalytic efficiency in existing PC systems are under considerable challenges. Herein, we report a metal modulation strategy that markedly improves the catalytic performance, represented by a series of metalloporphyrin complexes named M-TCPPs (M = Zn, Mn, Ni, Co, Cu). Zn-TCPP stands out an outstanding photocatalytic activity in the oxidation of nicotinamide adenine dinucleotide (NADH), nicotinamide adenine dinucleotide phosphate (NADPH), and certain amino acids. Significantly, in contrast to previously reported PCs involved in reductive cycles, Zn-TCPP undergoes an efficient oxidative cycle, which gives an amplified catalytic process. Furthermore, theoretical calculations suggest Zn-TCPP's superior photocatalytic performance occurred due to heightened intersystem crossing rates and geometry alterations. Also, in vitro investigations, both in G98T cells and multicellular spheroids, illuminated that Zn-TCPP has a therapeutic potential for photocatalytic antitumor therapy. This research highlights the function of "metal modulation" in developing high-performance PCs, and further motivates to refine PCs through the underlying principles of Zn-TCPP's design approach.

Poster Presentation : **ORGN.P-256**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Mechanistic study on enantioselective [(2+2)+2] cycloaddition

Donghun Hwang, Mu-Hyun Baik[1,*]

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

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

Highly ordered reactions with transition metal represented by [m+n+o] reaction have emerged as a platform towards cyclic motifs. In 2016, Baik and Evans reported [(2+2)+2] cycloaddition of tethered enyne with the chloroethyne was utilized to achieve one-step formation of 6-membered ring and stereogenic center. Recently, the Evans group successfully designed [(2+2)+2] cycloaddition of tethered enyne with 1-ethoxyethyne, where the alkyne was functionalized with an electron-donating group. In this study, we tried to investigate the mechanistic features with the combinatorial effort of experiment and computation, focusing on revealing the enantio, regio, and rate-determining step.

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Poster Presentation : **ORGN.P-257**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

NHC-Catalyzed Synthesis of Ketone from Xanthate through Photoinduced Electron Transfer

Sungwoo Hong[*], Minseok Kim

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

Given the widespread occurrence of alcohols and carboxylic acids, the potential utility of their fragment cross-coupling reactions in organic synthesis are substantial. Herein, we present a versatile technique for the synthesis of a broad spectrum of ketones from alcohols and carboxylic acid derivatives, facilitated by N-heterocyclic carbene (NHC) catalysis. Mechanistic investigations revealed that photoexcited xanthates undergo single electron transfer with acyl azoliums under photocatalyst-free conditions, generating NHC-derived ketyl radicals and alkyl radicals. These radical intermediates undergo the radical-radical cross-coupling reactions, resulting in the formation of valuable ketones. Additionally, this methodology extends to three-component reactions involving alkenes and enynes, leading to the production of structurally diverse cross-coupled ketones. This integrated approach provides a distinctive avenue for the fragment coupling of various alcohols and carboxylic acid derivatives, accommodating diverse functional groups.

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Poster Presentation : **ORGN.P-258**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Biorthogonal Activable Photocatalyst for Advanced Cancer Therapy

Jungryun Kim, Jusung An, Hyeonji Rha, Eunji Kim, Ki-ppeum Lee, Changyu Yoon, Huiyeon Moon, Yujin Kim, Yubin Lee, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Photodynamic Therapy (PDT) holds promise as a non-invasive and low-resistance antitumoral treatment with fewer side effects than alternatives; however, its limited efficacy in hypoxic conditions, prevalent in oxygen-deficient cancer cells due to rapid proliferation, remains a significant challenge. This study introduces a novel photoredox catalyst designed for advanced antitumoral phototherapy. The catalyst, activated through a biorthogonal Inverse electron-demand Diels–Alder reaction (IEDDA) reaction between the attached tetrazine moiety and Trans-cyclooctene (TCO), is conjugated with a ligand for specific mitochondria targeting. Through harnessing these reactions, the photocatalyst can specifically gather in cancer cells' mitochondria, and upon activation, it induces the oxidation of NADH to NAD+ for the targeted eradication of tumors. Overcoming the hypoxia challenge in cancer cells, this oxygen-independent therapeutic agent demonstrates bioorthogonal activation with precise targeting, offering a potential avenue for developing effective and selective photosensitive treatments.

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Poster Presentation : **ORGN.P-259**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Optimization of Chalcogen Element on Metal-free Photoredox Catalyst for Aggravated NADH/NAD+ Imbalance in Cell.

Eunji Kim, Jusung An, Jungryun Kim, Hyeonji Rha, Jaewon Kim, Changyu Yoon, Huiyeon Moon, Yujin Kim, Jiyoung Yoo, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Photoredox catalysis has proposed additional implement above the photodynamic therapy by oxygen independence, simple regulation, and successive apoptotic cascade reaction through electron transfer chain interruption. Metal ion, such as Ir, or Ru complex demonstrated high performance of photoredox behavior in methodology triggered by light, yet few metal-free catalysts were reported in biological environment. The attempts effectively killed the cancer, but it accommodated intrinsic metabolic toxicity. For example, metal complex verified such a powerful redox cycle that it latent for several side reactions. Few organic photoredox catalyst (PC) already demonstrated redox competence on uncaging strategy through tetrazine oxidation but demands still exist for the relevant field in terms of diversity and efficiency development of catalyst. In this research, we suggest the chalcogen element substitution strategy to elucidate the anticancer photosensitizer design of metal-free photoredox catalyst. Our compound employed rhodamine backbone by replacing hetero atom to oxygen, sulfur, and selenium and were designed to arouse NADH/NAD+ imbalance. For the sake of bioorthogonality, we propose the design strategy for metal-free photoredox catalyst in a mild condition and verify the anticancer effect in cell.

Poster Presentation : **ORGN.P-260**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Observing lipid droplets to detect changes with a fluorogenic probe

Bokyeong Hwang, Juyoung Yoon*, Hwan Myung Kim[1,*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1] *Department of Energy Systems Research, Ajou University, Korea*

Lipid droplets (LDs) play a crucial role in storing cellular lipids within cells and are closely associated with various biological processes and metabolic disorders. Understanding the dynamic changes of LDs is essential for addressing issues related to energy storage and human health. Monitoring the dynamic changes in early hepatic steatosis requires the use of LD probes.Fluorescence microscopy has been widely employed for evaluating membrane organelles due to its high sensitivity, precision, and rapid acquisition. Chemical targeting based on cellular microenvironment factors such as polarity, temperature and small molecules is achieved using specific probes. Excited-state intramolecular proton transfer is utilized in dynamic imaging of LDs, providing sensitivity to environmental factors except for polarity. The ideal LD fluorogenic probe should possess good biocompatibility, high lipid specificity, and brightness for tracking the polarity alteration of LDs during hepatic steatosis.Organic dyes with donor–acceptor structures exhibit selective staining of LDs. The donor–acceptor structures, characterized by a distinct charge transfer process, typically show weak fluorescence in polar solvents, indicating high sensitivity to polarity changes. Based on this principle, LD-specific fluorogenic probe, LD-1, was designed to detect variations in LDs in cells and tissues over time, reflecting hepatic steatosis. The results suggest that these polarity-sensitive and commercially viable LD probes could be extended to track LD origins and interactions with enzymes or enzyme mimics in the future.

Poster Presentation : **ORGN.P-261**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Colorimetric and Fluorometric Bimodal Amine Chemosensor for Detection of Food Spoilage

Seon Young Park, Na Young Cho, Eun Hye Lee, Jong Hyun Kim[*]

Department of Molecular Science and Technology, Ajou University, Korea

Amine derivatives are generated from spoiled protein foods which cause foodborne diseases. Therefore, sensitive detection of amine derivatives is highly desired. In this presentation, a new chemosensor (DEAH) is introduced being capable of detecting which is based on colorimetric and fluorometric bimodal sensing. DEAH solution exhibits discernible color changes with high sensitivity (limit of detection: 36.9nM), selectivity, and rapid detection time (< 1s) in response to amine derivatives. DEAH films also shows a clear color change from yellow to violet ($\triangle E_{ab} > 98$) and turn-on fluorescence when exposed to amine derivatives. Based on versatile applicability of DEAH, we successfully demonstrated effective bimodal detection of amine derivatives using DEAH in solutions, solids, and films, and real-time monitoring of food quality using DEAH-coated films.

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Poster Presentation : **ORGN.P-262**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Water-soluble H_2S chemosensor harnessing colorimetric redox property of indigo dye

Eun Hye Lee, Jong Hyun Kim*

Department of Molecular Science and Technology, Ajou University, Korea

In this presentation, we report a water-soluble colorimetric H_2S chemosensor (ID) using indigo dye. Taking advantages of colorimetric redox reaction, we selected indigo as chemosensor backbone while pyridinium unit was attatched to endow with water-solubility. ID exhibits efficient color changes from blue to white in reponse to H_2S through the redox reaction. Moreover, ID features versatility in detection conditions, by showing H_2S detection in solution and dyed films, suggesting practical applicability in various environments.

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Poster Presentation : **ORGN.P-263**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthetic Approaches towards Tetrahydrobenzazepines via Intramolecular Oxidative Aza-Prins type Cyclization

Hyuckin Kwon, Sun-Joon Min[1,*]

Applied chemistry, Hanyang University, Korea

[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Cephalotaxus alkaloids are the first alkaloids characterized from the fruits and leaves of C. harringtonia, the only genus of the Cephalotaxaceae family, which consists of eleven species of small, evergreen plants. Their unique core structure consists of tetrahydrobenzazepine fused with an azaspirononane unit, which has prompted an interest in the isolation, characterization, biological evaluation, and overall synthesis of cephalotaxus alkaloids and analogues. For instance, homoharringtonine (HHT), known as omacetaxine, a simple ester of cephalotaxine, is in clinical development by the National Cancer Institute (NCI) because it is easy to purify and most abundant in plants. In particular, a mixture of harringtonine (HT) with HHT have been used in traditional Chinese medicine (TCM) to treat a variety of malignancies. Up to date, a number of synthetic approaches towards cephalotaxus alkaloids have been reported. While most synthetic routes to the core ring structures have been studied based on an intramolecular Mannich cyclization using Lewis acids, the development of new synthetic methods for this class of alkaloids under metal free conditions are still challenging. Herein, we report our efforts to synthesize cephalotaxus alkaloid's core structure via intramolecular oxidative aza-Prins type cyclization. This presentation will focus on a selective reduction of propargylsilane to Z-allylsilane and an intramolecular cyclization of the corresponding advanced allylsilanes to construct tetrahydrobenzazepine scaffolds under visible-light irradiation in the presence of photoredox catalysts.

Poster Presentation : **ORGN.P-264**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Enzyme-Instructed Intramitochondrial Polymerization for Enhanced Anticancer Treatment without the Development of Drug-Resistance

Sangpil Kim, Ja-Hyoung Ryu[1,*]

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

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Intracellular polymerization in living cells motivated chemists to generate polymeric structures with a multitude of possibilities to interact with biomacromolecules. However, out-of-control of the intracellular chemical reactions would be an obstacle restricting its application, providing the toxicity of non-targeted cells. Here, we reported intracellular thioesterase-mediated polymerization for selectively occurring polymerization using disulfide bonds in cancer cells. The acetylated monomers did not form disulfide bonds even under an oxidative environment, but they could polymerize into the polymeric structure after cleavage of acetyl groups only when encountered activity of thioesterase enzyme. Since thioesterase enzymes were overexpressed in cancer cells specifically, the polymerization could occur selectively in the cancer mitochondria. The resulting polymeric structures disrupted the mitochondrial membrane, thus activating the cellular death of cancer cells with high selectivity. This strategy selectively targets diverse cancer cells involving drug-resistant cells over normal cells. Moreover, the mitochondria targeting strategy overcomes the development of drug resistance even with repeated treatment. This approach provides a way for selective intracellular polymerization with desirable anticancer treatment.

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Poster Presentation : **ORGN.P-265**

Organic Chemistry

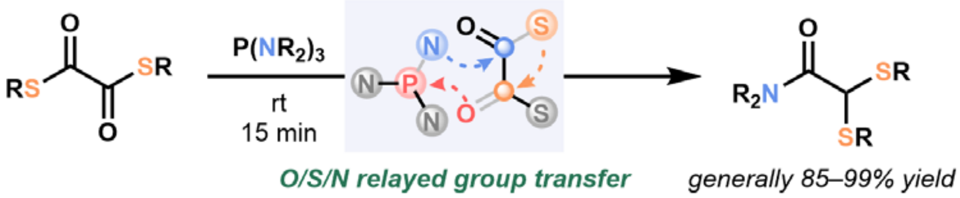
Exhibition Hall 2 FRI 11:00~13:00

Relayed Heteroatom Group Transfer: A Structural Reorganization between Bisthioester and Triaminophosphine to α,α-Disulfenylamide

Ilju Jeong, Jun-Ho Choi*, Won-jin Chung*

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

Simultaneous multiple displacements of organic molecules can lead to a large structural reconstruction with increased complexity that would be difficult to access otherwise. Whereas double displacement such as olefin metathesis is well-established, higher-order versions remain much more challenging, because of their intrinsic thermodynamic disadvantages. Here, we describe a newly discovered relayed heteroatom group transfer process between bisthioesters and triaminophosphines as an unusual example of a formal triple displacement. Through the oxygen/nitrogen exchange between the two simple starting materials, in addition to the 1,2-sulfur migration of a putative carbene intermediate, an organized relocation of the O/S/N groups proceeded to give a variety of α,α-disulfenylamides with excellent efficiency under ambient conditions. The experimental and computational mechanistic studies revealed the sequence of the relayed group shifts via an α,α-disulfenyl phosphonium enolate intermediate as well as the dual role of triaminophosphine as both an oxygen acceptor and a nitrogen donor.



- novel relayed heteroatom group transfer process
- TM/photocatalyst-free 1,2-sulfur migration
- unusual amino group transfer from phosphine
- rapid & highly efficient
- no steric & electronic constraints
- mechanistic study & DFT calculation

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Poster Presentation : **ORGN.P-266**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

All-in-one Organic Ligands for High Resolution Patterning of Perovskite Nanocrystals

Na Young Cho, Sangwook Kim[1], Jin Woo Choi[2], Jong Hyun Kim[*]

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[1]*Division of Applied Chemistry & Biological Enginee, Ajou University, Korea*
[2]*Kongju National University, Korea*

Perovskite nanocrystals (PNCs) have emerged as a promising light-emitting material owing to their facile tunability of wavelengths, excellent photoluminescence quantum yields and high color purity. However, photolithography-based patterning is incompatible with PNCs because of their vulnerable nature to polar solvents. Herein, we report functional organic ligands (AzL1, AzL2, AzL1-Th, AzL2-Th) being capable of photocrosslinking, PNC stabilizing, and charge transporting. In particular, AzL1-Th exhibited the highest efficiency of crosslink, improved photoluminescence quantum yields, and good charge mobility. Using AzL1-Th we successfully demonstrated highly emissive AzL1-Th-attached PNCs and effectively crosslinked perovskite LEDs.

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Poster Presentation : **ORGN.P-267**

Organic Chemistry

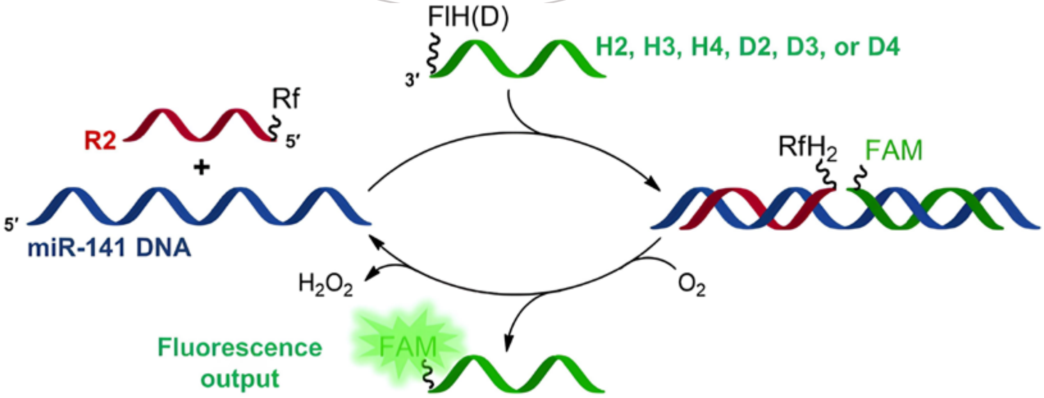
Exhibition Hall 2 FRI 11:00~13:00

Photooxidation of reduced FAM by riboflavin for nucleic acid templated reactions to detect miR-141

Yeojin Kim, Ki Tae Kim[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

Nucleic acid templated reactions enhance nucleic acid signals through chemical reactions. It is essential to develop reaction pairs that have high reaction speeds and low background signals so that nucleic acid signals can be quickly amplified using templated reactions. In this study, a new reaction pair of reduced 5(6)-carboxyfluorescein (FAM) and riboflavin was developed that shows low background levels. In the presence of riboflavin, reduced FAM returns to its original (fluorescent) form when exposed to blue light. Based on this reaction, a biosensor was developed that detected 100 pM of DNA (miR-141). Upon exposure to fluorescent light, FAM obtained from the nucleic acid templated reaction generated superoxide, which can oxidize 3,3'5,5'-tetramethylbenzidine (TMB), a visualizing reagent. Based on this oxidation, a color-change-based nucleic acid sensor was also developed.



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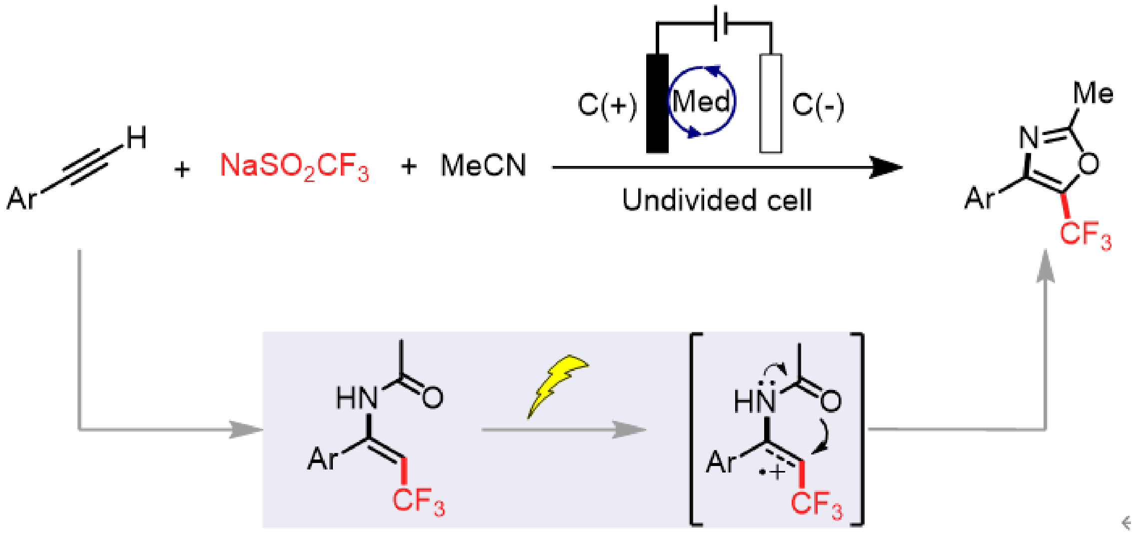
Poster Presentation : **ORGN.P-268**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Electrochemical synthesis of trifluoromethyl oxazoles through cascade aminotrifluoromethylation and cyclization of alkynes

Jihoon Jang

Chemistry, Chung-Ang University, Korea

Oxazoles are important compounds that are found in various natural products and pharmaceuticals, and exhibit unique biological activities. In particular, oxazoles that contain trifluoromethyl groups have attracted much attention because the introduction of fluorine atoms into pharmaceuticals and agrochemicals can favorably change their properties and biological activities. We propose a cascade electrochemical aminotrifluoromethylation and cyclization process of alkynes for the synthesis of trifluoromethyl oxazole derivatives. This process requires several oxidation steps, but by utilizing electrochemistry, it enables efficient synthesis without the need for oxidants. Additionally, through exquisite control of conditions, it minimizes side reactions and synthesizes the desired product with high yield.


Ar
H
+ $NaSO_2CF_3$ + MeCN
C(+)
Med
C(-)
Undivided cell
Me
N
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Poster Presentation : **ORGN.P-269**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of Pb^{2+} Sensor Based on G-quadruplex Complex with Modified Thioflavin T

<u>Duyeop Kim</u>, Ji Hoon Han[*]

Department of Chemical and Biological Engineering, Andong National University, Korea

Thioflavin T(ThT), a fluorescent molecular rotor, has been widely utilized for detecting G-quadruplexes, exhibiting remarkable light-up fluorescence intensity due to the restriction of rotation. As a feature for switching G-quadruplex topology, several Pb^{2+} sensors using the G-quadruplex/ThT complex have been developed. However, there are few cases of turn-on fluorescent biosensors utilizing the G-quadruplex/ThT complex. In this study, we aim to develop a fluorescent light-up sensor for the detection of Pb^{2+}. Our newly synthesized ThT derivatives, modified at the *N*3 position on the benzothiazole ring and the *N* of aniline, with the T2 G-quadruplex, show fluorescent light-up upon the addition of Pb^{2+}. Particularly, G-quadruplexes with ThT-E or ThT-P exhibit significant fluorescent light-up properties. Furthermore, our sensor demonstrated high selectivity against several different toxic metal ions. Thus, our sensor shows potential application for monitoring Pb^{2+} in environmental samples.

Poster Presentation : **ORGN.P-270**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Redox-Active and Fluorescent Benzenes: Bipolar Small Molecules for Symmetric Redox Flow Batteries

Younghun Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Bipolar redox-active organic molecules (ROMs) can simplify the manufacturing process to fabricate cost-effective symmetric all-organic batteries. Symmetric cells are even more advantageous, particularly when implemented as redox flow batteries (RFBs), since they do not suffer from detrimental crossover issues that lead to capacity fading. The development of bipolar ROMs, however, needs to overcome the synthetic challenge of incorporating both *n*-type and *p*-type redox-active motifs (or even radicals) within a single molecule. In this context, single-benzene fluorophores (SBFs) serve as an excellent starting point since they have both electron-withdrawing groups (EWGs) and electron-donating groups (EDGs) conjugated across the benzene core. To realize this idea, we are exploring single-benzene redoxphores (SBRs) as a new class of bipolar ROMs. These SBRs feature 1,4-diacetylbenzene as the reduction site, and p-phenylenediamine or hydroquinone as the oxidation site residing together within a single benzene platform. By substituting acidic protons of the amino or hydroxy groups with oligoether chains, both the reversibility of redox reactions and the solubility in electrolytes were significantly improved. Built upon a SBF motif, SBRs can also report the state-of-health (SOH) of the electrochemical cells by changes in light-emitting properties. This presentation will discuss a new design strategy for developing fluorescent bipolar ROMs and their technological applications in symmetric RFBs.

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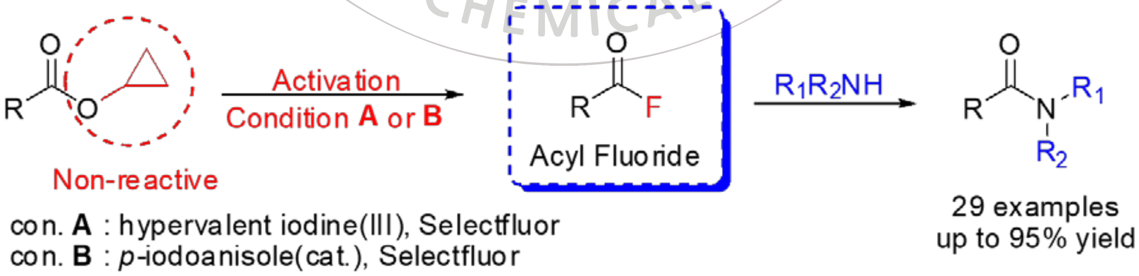
Poster Presentation : **ORGN.P-271**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Catalytic Activation of Deactivated Cyclopropyl Esters using Hypervalent Iodine(III) and Selectfluor

Eunsol Choi, Hyo-Jun Lee[1,*]

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

The transformation of alkyl ester is very useful for efficient synthesis of target compounds. However, harsh reaction conditions and metallic reagents are required. Here we report cyclopropyl ester activation using hypervalent iodine(III) and Selectfluor to generate acyl fluoride intermediates that can be smoothly modified into various functional groups depending on the types of nucleophile. Furthermore, we investigated a protocol enabling the in-situ generation of hypervalent iodine(III) using catalytic amounts of a 4-iodoanisole and Selectfluor for even more efficient, environmentally friendly, and atom-economical approach.



133rd General Meeting of the Korean Chemical Society

April 24(Wed)~26(Fri), 2024, Suwon Convention Center, Korea

Poster Presentation : **ORGN.P-272**

Organic Chemistry

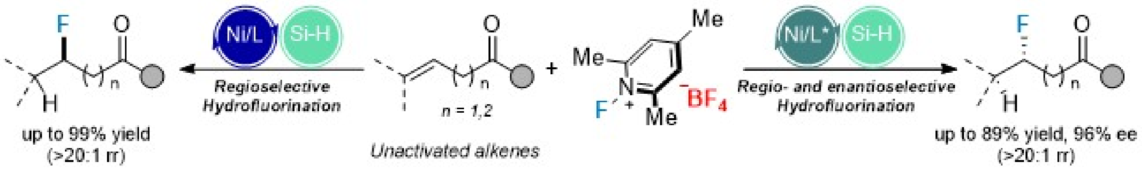
Exhibition Hall 2 FRI 11:00~13:00

Nickel-Catalyzed Regio-and Enantioselective Hydrofluorination of Unactivated Alkenes.

Seunghoon Han, **Sungwoo Hong***

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

The development of regio- and enantioselective C–F bonds from easily accessible alkenes represents a significant challenge in organic synthesis. In our study, we present a method for selectively forming C–F bonds using nickel hydride catalysis and a coordination-directed strategy. This approach allows for precise hydrofluorination of both terminal and internal alkenes. Notably, we have fine-tuned this technique to achieve high levels of enantioselectivity in generating aliphatic C–F stereogenic centers by employing a tailored chiral ligand. Furthermore, our research highlights the discovery of the (+)-non-linear effect under optimized conditions, enabling substantial enantioselectivity even with moderately enantiomerically enriched chiral ligands. Given fluorine's crucial role in pharmaceuticals and synthetic materials, our findings provide valuable insights into the regio- and enantioselective formation of C–F bonds, facilitating the efficient synthesis of important fluorinated compounds.



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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **ORGN.P-273**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Crystallization-Induced Chiral Recognition of Short β-Peptide Foldamers in Racemic Mixtures

Seoneun Jeong, Jintaek Gong[1], Woo youn Kim[2], Hee-Seung Lee[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemistry Education, Sunchon National University, Korea*
[2]*Department of Chemistry, KAIST, Korea*

Chirality is a fundamental aspect of nature and plays a pivotal role in the structure and dynamics of proteins and other biomolecules. The inherent chirality of L-enantiomers in amino acids essential to protein composition exemplifies this phenomenon. This property leads to self-sorting behaviors widely observed in biological systems. Despite its importance, the mechanisms of self-recognition and self-discrimination in chiral systems are not fully understood, highlighting the need for research using simpler models.Our study focuses on the synthesis of β-peptide foldamers, incorporating either (*R*,*R*)- or (*S*,*S*)-*trans*-2-aminocyclopentanecarboxylic acid (ACPC) and capped with pyridyl groups. These foldamers are crucial for investigating metal-induced crystallization, an approach that aids in studying chiral recognition and discrimination in coordination chains. X-ray diffraction analyses have demonstrated that the tendencies for heterochiral and homochiral coordination are influenced by the length of the chiral ligand and the specific conditions under which the crystals grow. Furthermore, the protein–ligand interaction profiler (PLIP) has been instrumental in elucidating the intermolecular interactions within homochiral configurations, which are key to understanding the formation of racemic mixtures' structures. Our examination of these mixtures of varied chiral molecules is poised to provide critical insights, potentially illuminating aspects of the origin of life in future studies.

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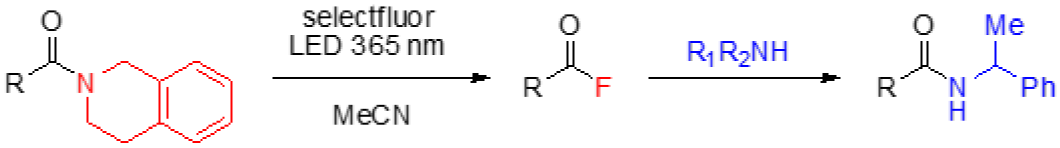
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Exploring the Versatility of Tetrahydroisoquinoline : Efficient Method for Amide Activation

Yelin Han, Hyo-Jun Lee[1,*]

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

Amides are extensively utilized in our life and play crucial roles in the natural and chemical industrial fields. However, conversion amides into alternative compounds has been challenging due to its low reactivity. Herein, we propose a method to generate acyl fluoride intermediates via cleavage of the C-N bond of amides having 1,2,3,4-tetrahydroisoquinoline units, under mild and metal-free conditions. The resulting versatile acyl fluoride intermediates can be converted into diverse functional groups depending on nucleophilic preferences. This research will contribute to the diverse applications of amide compounds.



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Poster Presentation : **ORGN.P-275**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

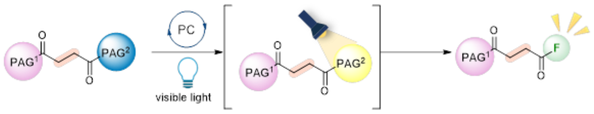
Photoredox catalyzed chemoselective activation of p-methoxybenzyl ester for generation of actl fluoride

<u>HeeChan Jeong</u>, Hyo-Jun Lee[1,*]

chemistry, Kunsan National University, Korea

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

Recently, there has been a significant focus on achieving chemoselective activation of specific functional groups, aiming to streamline synthetic processes in the production of industrial materials while prioritizing environmental friendliness. Various methodologies have been developed utilizing metal catalysts and metal reagents while the development of chemoselective activation under metal-free conditions is barely reported. Herein, we have developed the chemoselective activation of p-methoxy benzyl (PMB) esters utilizing the highly reactive benzylic proton in the presence of photoredox organocatalyst. We anticipate that this protocol will significantly contribute to pharmaceutical and agrochemical industry.


PAG¹
O
O
PAG²
PC
visible light
PAG¹
O
O
PAG²
PAG¹
O
O
F

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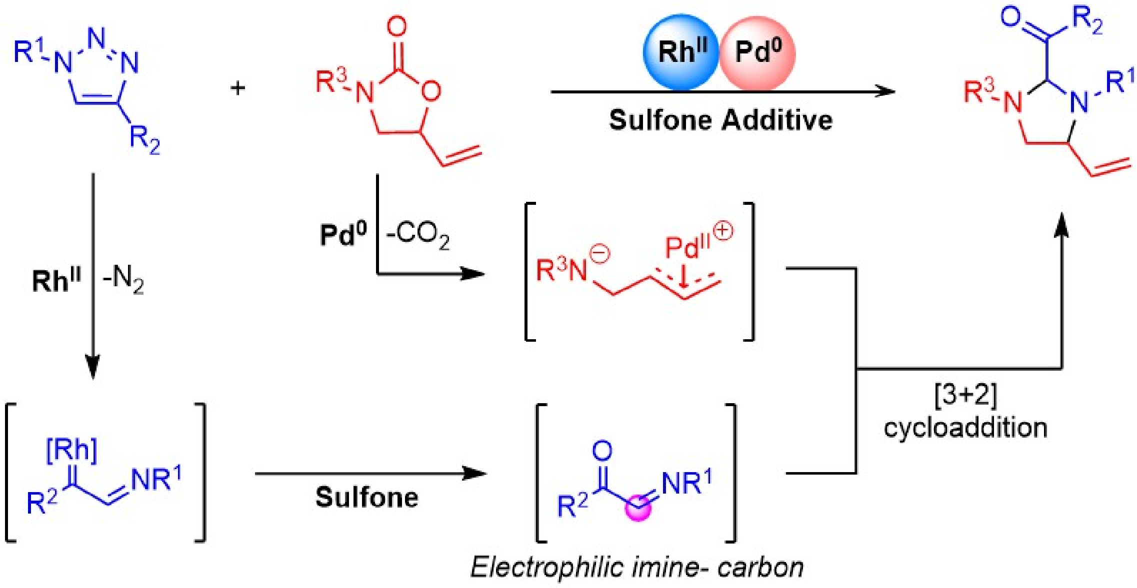
Poster Presentation : **ORGN.P-276**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Dual Rh(II)/Pd(0)-Catalyzed [3+2] Cycloadditions between Electrophilic Imine of α-Imino Rh(II)-Carbenoids with π-Allyl Pd(II)-Complex

Soha Yang, Yu Lim Lee, Juri Kim, Sang-gi Lee*

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

Dual catalysis has emerged as a powerful tool to synthesize a diverse range of organic compounds which cannot be achieved with traditional single-metal catalysis. Recently, we have established a cooperative Pd(0)/Rh(II) dual-catalytic system, employing allylic substrates and N-sulfonyl-1,2,3-triazoles as precursors of π-allyl Pd(II)-complex and N-nucleophilic/C-electrophilic α-imino metal-carbenoid intermediates. However, there are no examples on utilizing the electrophilic nature of the imine of metal-carbenoids. Herein, we report an unprecedented catalytic reaction between the α-imino Rh(II)-carbenoids and π-allyl Pd(II)-complex intermediates, involving intermolecular oxygen transfer from sulfone into the Rh(II)-carbenoid carbon, which could induce the imine moiety as the reactive electrophilic functional group, i.e., in the presence of sulfone additive, the Rh(II)-carbenoid intermediate has been oxidized first, and then the imine moiety undergoes [3+2] cycloaddition reaction with the π-allyl Pd(II)-complex to afford an imidazolidin-2-yl ketone ring.


RhII
Pd0
Sulfone Additive
RhII -N2
Pd0 -CO2
Sulfone
[3+2] cycloaddition
Electrophilic imine- carbon

Poster Presentation : **ORGN.P-277**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Thioamide β-Peptide: Secondary Structure Regulation and Post-synthetic Modification

Jungwoo Hong, **Hee-Seung Lee***

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

Amide functionality plays a vital role in living organisms and organic chemistry, prompting interest in the development of bioisosteres that mimic its structural and functional characteristics. Among various amide bioisosteres, thioamide stands out due to its advantageous properties, including enzymatic tolerance, hydrogen bonding capability, versatile reactivity, spectroscopic labeling, and photoisomerism. Despite these merits, there is a notable scarcity of systematic studies focusing on peptides incorporating multiple thioamides, limiting a comprehensive exploration of their benefits.To address this gap, we have formulated and synthesized a series of β-peptides featuring thioamide residues. Intriguingly, our investigation revealed a novel and explicit correlation between the thioamide sequence and peptide secondary structure. Moreover, the enhanced reactivity of thioamide facilitates the regioselective and diverse embellishment of β-peptide. These findings emphasize the potential of thioamides as a promising component in the realm of organic, materials, and medicinal chemistry.

Poster Presentation : **ORGN.P-278**

Organic Chemistry

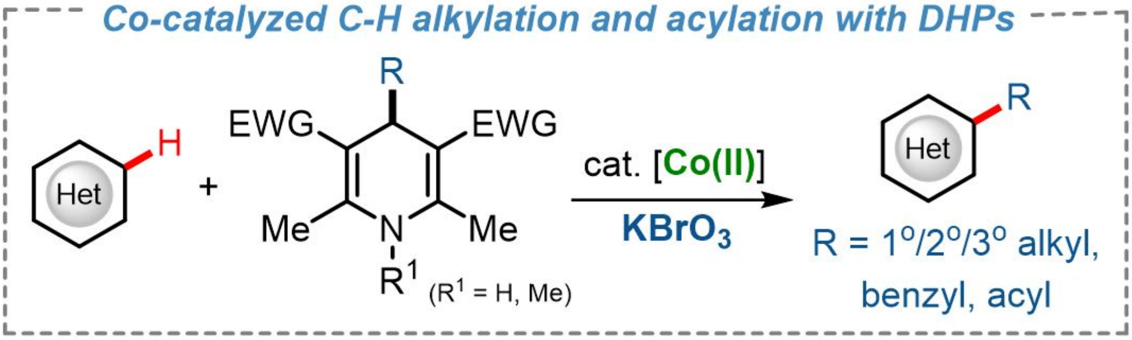
Exhibition Hall 2 FRI 11:00~13:00

Cobalt(II) Catalyzed C−H Alkylation of Various *N*-Heterocycles with 1,4-Dihydropyridines

Kyeongwon Moon, **In Su Kim***

School of Pharmacy, Sungkyunkwan University, Korea

The rapid incorporation of alkyl and acyl groups into C−H bonds of *N*-heterocycles is in demand for the development of lead candidates in drug discovery. Notably, a combination of $KBrO_3$ and Co(II) catalyst was successfully employed for the generation of alkyl and acyl radicals from DHPs. A series of heterocycles including azauracils, quinoxalinones, pyrazinones, pyridones, quinolones, quinazolinones, xanthines, chromones, and azine *N*-oxides were compatible under the developed conditions. Additionally, new azauracil derivatives were created using various 1,4-dihydropyridines. Combined mechanistic investigations aided the elucidation of a plausible reaction mechanism.



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Poster Presentation : **ORGN.P-279**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

AIE-based fluorescent probe to detect peroxynitrite levels in human serum and its cellular imagings

Jiyoung Yoo, Jaewon Kim, Jusung An, Jungryun Kim, Hyeonji Rha, Eunji Kim, Yujin Kim, Changyu Yoon, Huiyeon Moon, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

An AIE-based fluorescent probe was designed to evaluate peroxynitrite levels in complex biological samples. We have newly synthesized hydrazone-conjugated probe able to give a strong fluorescence in the presence of peroxynitrite. Regarding clinical application, we could measure the peroxynitrite levels both in human serum and in cellular mitochondria as LOD of 6.5 nM by fluorescence imaging in vitro.

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Poster Presentation : **ORGN.P-280**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Ir(triNHC)-Catalyzed Synthesis of α-Hydroxy Acids Using Glycerol

Jaeho Kim, Hye-Young Jang[1,*]

Department of Energy Systems Research, Ajou University, Korea

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

Glycerol, a biomass derivative, possesses advantages such as non-toxicity and biodegradability. Due to these advantages, numerous studies are being conducted on the utilization of glycerol. Generally, dehydrogenated glycerol readily undergoes the Cannizzaro reaction, leading to the conversion into lactic acid rather than forming C-C bonds. In this study, we successfully synthesized industrially valuable α-hydroxy acids (AHAs) through dehydrogenation reactions using triNHC-iridium catalysts, enabling the formation of C-C bonds between glycerol and various alcohols. As a result, we were able to effectively synthesize compounds with extended carbon chains from glycerol. We proposed a plausible mechanism using ESI-Mass and NMR spectroscopy.

Poster Presentation : **ORGN.P-281**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Photoinduced Atom-Transfer-Radical-Addition(ATRA) of Ortho-Amino Arylalkynes: De novo synthesis of Fluorinated Quinolines

Taehyun Oh, Chulbom Lee[*], Eun Jin Cho[1,*]

Division of Chemistry, Seoul National University, Korea

[1]*Department of Chemistry, Chung-Ang University, Korea*

The atom-transfer-radical addition(ATRA) of 2-alkynylanilines and CFBr3 has been developed using N-methylmorpholine(NMM) and photonic energy in a mild condition. Under visible light irradiation, photoinduced charge transfer of a CFBr3–NMM halogen bond (XB) complex generate •CFBr2 and •Br–NMM radicals, which undergo alkyne addition and halogen atom transfer (XAT) to furnish the atom-transfer radical addition (ATRA) product en route aromatization. With a broad substrate scope, the new reaction not only represents novel de novo entry to 2-fluorinated quinolines but also yields quinoline building blocks possessing 2,4-dihalides that can be converted to a variety of other quinolines.

Poster Presentation : **ORGN.P-282**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Dual Emissive Tetrathiafulvalene Mono-sulfoxides

Ye jin Kim, Jung Su Park[*]

Department of Chemistry, Sookmyung Women's University, Korea

TTF (Tetrathiafulvalene) and its derivatives have received tremendous attention in various fields of material science for various applications, including optical materials, photovoltaic solar cells, organic field-effect transistors, and sensors. As a result, numerous TTF and related derivatives were synthesized and studied for various target applications. However, there has been little effort to synthesize their oxidation products, hereby tetrathiafulvalene-sulfoxide derivatives and study their relevant properties. Here, we report the synthesis of a series of the TTF-mono sulfoxide derivatives, obtaining from m-CPBA oxidation of quinoxaline-annulated TTF frameworks. We also studied the photophysical and electrochemical properties of these sulfoxide derivative. Unexpectedly, these TTF-mono-sulfoxide derivative in common display a very interesting dual emissive property, which can be further characterized as the combination of localized emission (LE) and intramolecular charge transfer (ICT) emission. These dual emission properties are very sensitive to the solvent polarity and water content in organic solvents. Here, the details of the synthesis, characterization, photochemical and electrochemical properties, and ratiometric sensing properties of these materials will be discussed.

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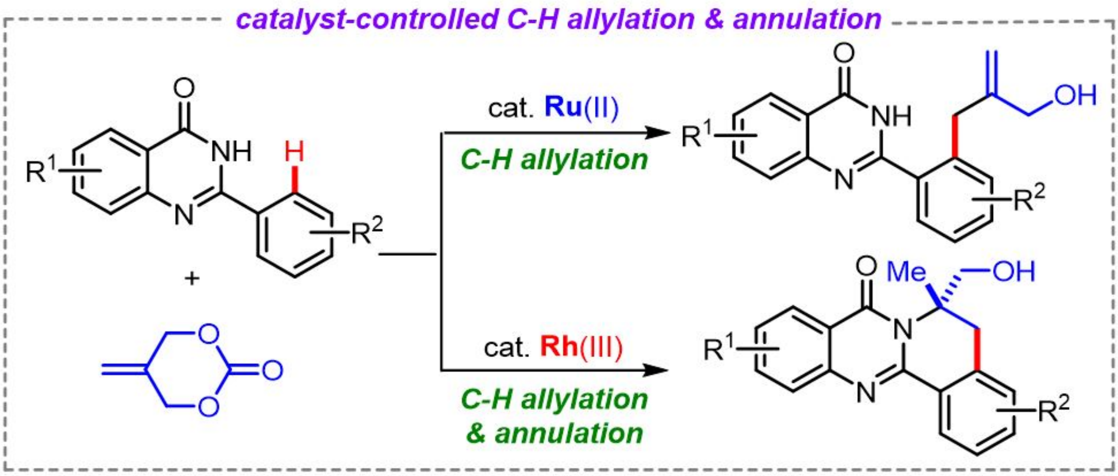
Poster Presentation : **ORGN.P-283**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Catalyst-Controlled C–H Allylation and Annulation of Quinazolinones with 2-Methylidene Cyclic Carbonate

Heesang Yang, In Su Kim*

School of Pharmacy, Sungkyunkwan University, Korea

The site-selective modification of quinazolinone as a privileged bicyclic *N*-heterocycle is an attractive topic in medicinal chemistry and material science. We herein report the ruthenium(II)-catalyzed C–H allylation of 2-aryl quinazolinones with 2-methylidene cyclic carbonate. In addition, tandem C–H allylation and annulation are achieved under rhodium(III) catalysis, resulting in the formation of tetracyclic quinazolinones including a tertiary carbon center. Post-transformations of the synthesized products demonstrate the potential of the developed methodology. A series of mechanistic investigations were also performed.



Poster Presentation : **ORGN.P-284**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Intramolecular hydroamidation of alkenes enabling asymmetric synthesis of β-lactams via transposed NiH catalysis

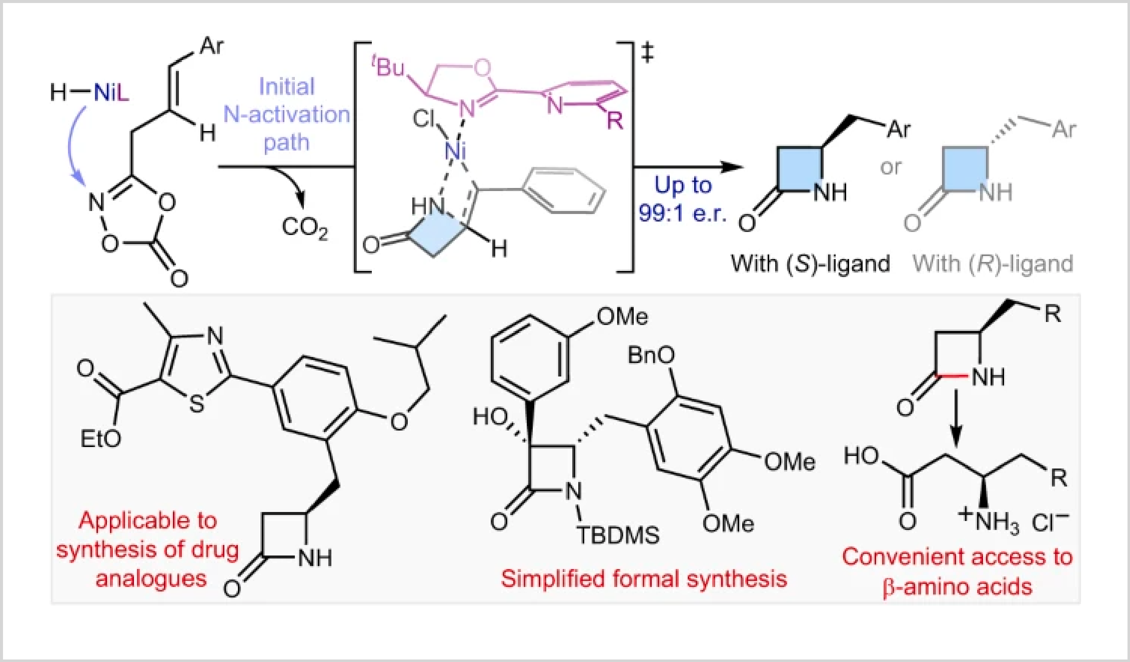
Xiang Lyu, Sangwon Seo[1,*], Sukbok Chang[2,*]

Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, China

[1]*Department of Physics and Chemistry, Daegu Gyeongbuk Institute of Science & Technology, Korea*

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

Synthetic methods for constructing enantioenriched β-lactams are highly valuable given their ubiquity in bioactive compounds, most notably in antibiotics such as penicillins and carbapenems. Intramolecular hydroamidation of β,γ-unsaturated amides would provide a convenient means to reach this alluring chemical space, yet it remains limited due to the regioselectivity issue arising from the difficulty associated with the formation of strained four-membered rings. Here we describe a NiH-catalysed strategy that addresses this challenge through the use of readily accessible alkenyl dioxazolone derivatives. The reaction transcends the conventional NiH operation mode via a transposed mechanism initiated by N-activation, thus allowing for proximal C–N bond formation with excellent regioselectivity, regardless of the electronic properties of substituents. This mechanistic platform is also highly effective for the enantioselective intramolecular hydroamidation of alkenes to enable convenient access to enantioenriched β-lactams.


H—NiL
Ar
H
Initial
N-activation
path
CO2
tBu
Cl
Ni
HN
H
‡
Up to
99:1 e.r.
Ar
NH
or
With (S)-ligand
With (R)-ligand
EtO
Applicable to
synthesis of drug
analogues
OMe
BnO
HO
TBDMS
Simplified formal synthesis
R
HO
+NH3 Cl−
Convenient access to
β-amino acids

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Poster Presentation : **ORGN.P-285**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Visible-light-promoted Nickel-Catalyzed carbofunctionalization of Alkynes

Soyeon Sung, Yong Ho Lee[*]

Department of Chemistry, Korea University, Korea

Visible light photoredox catalysis has emerged as a powerful strategy for the activation of small molecules and the synthesis of valuable materials, offering environmentally friendly and efficient synthetic routes. In this work, we present a novel approach to carbofunctionalization, utilizing a Ni-photocatalysis system activated by visible light. This method employs readily available building blocks, demonstrating the versatility and accessibility of our reaction for synthesizing complex value-added molecules.

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Poster Presentation : **ORGN.P-286**

Organic Chemistry

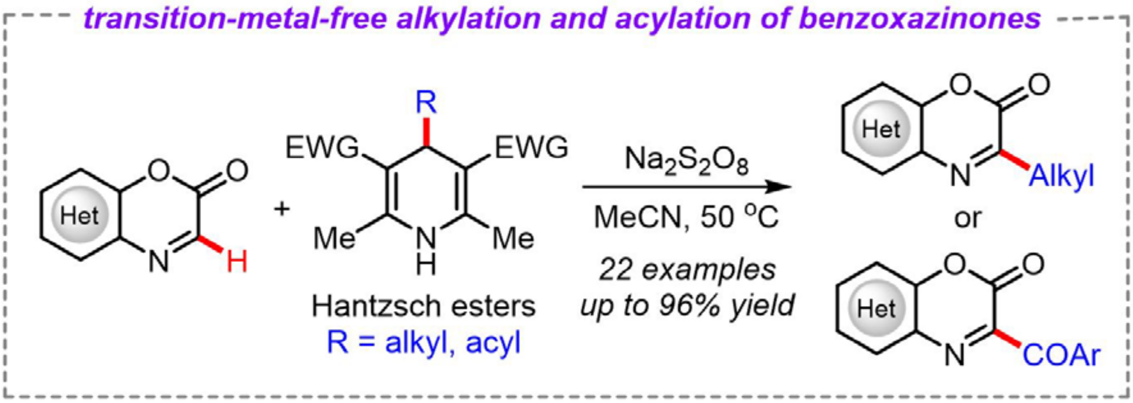
Exhibition Hall 2 FRI 11:00~13:00

Transition-Metal-Free C−H Activation of Benzoxazinones with Hantzsch Esters

Hyungjin Shin, In Su Kim*

School of Pharmacy, Sungkyunkwan University, Korea

The direct functionalization of *N*-heterocycles is a vital transformation for the development of pharmaceuticals, functional materials, and other chemical entities. Herein, the transition-metal-free alkylation and acylation of $C(sp^2)$−H bonds in biologically relevant 2-benzoxazinones with 1,4-dihydropyridines as readily accessible radical surrogates is described. Excellent functional group compatibility and a broad substrate scope were attained. Gram-scale reaction and transformations of the synthesized adducts via Suzuki coupling with heteroaryl boronic acids demonstrated the synthetic potential of the developed protocol.



Poster Presentation : **ORGN.P-287**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Efficient three component coupling reactions utilizing arynes, phosphites, and silyl fluorides for the synthesis of ortho-silylated arylphosphonate

Suhyun Ji

Sogang University, Korea

A mild, efficient, and metal-free three component coupling reaction involving arynes, phosphites, and fluorosilanes was developed to afford ortho-silylated arylphosphonate. Despite the formidable bond energy inherent in Si-F, our reaction effectively activated it, thereby facilitating the incorporation of a silyl group at the ortho position. The reaction proceeded well with a wide array of silyl fluoride variants. Moreover, the reaction is tolerant to various functional groups, providing diverse ortho-silylated arylphosphonate in moderate to good yields.

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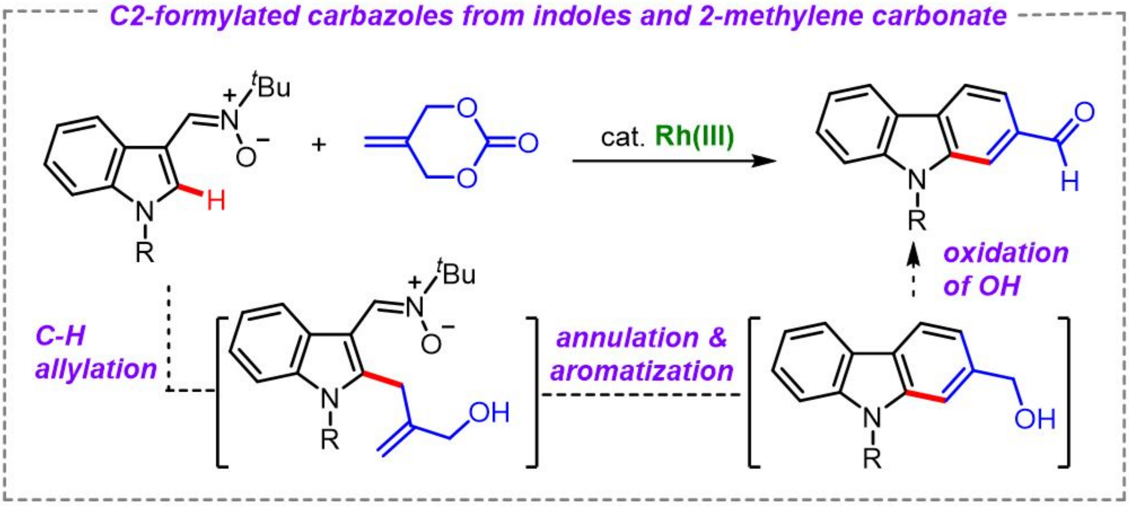
Poster Presentation : **ORGN.P-288**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis of 2-Formyl Carbazoles: C−H Allylation & Cyclization of Nitrones with 2-Methylidene Cyclic Carbonate

Sujin Min, In Su Kim[*]

School of Pharmacy, Sungkyunkwan University, Korea

The synthesis of functionalized carbazoles as privileged nitrogen heterocycles has emerged as a central topic in drug discovery and material science. We herein disclose the Rhodium(III)-catalyzed cross-coupling reaction between indolyl nitrones and 2-methylidene cyclic carbonate as an allylating surrogate, resulting in the formation of C2-formylated carbazoles via tandem C−H allylation, [3+2] cycloaddition, aromatization and benzylic oxidation. The synthetic utility of this protocol is highlighted by a variety of post-transformation of C2-formylated carbazoles.



Poster Presentation : **ORGN.P-289**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of benzophenone derivatives using acylsilanes via palladium-catalyzed coupling reactions

Jaehoon Lee, Inji Shin*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Diarylketones serve as important building blocks in natural products and synthetic intermediates. Benzophenone, the simplest form of diarylketones, possesses diverse properties with wide-ranging applications. Functionally modified benzophenones play essential roles in pharmaceutical synthesis, cosmetics, and UV absorbers, among other fields. This study explores a novel synthetic approach to generate various benzophenone derivatives. Transition-metal catalyzed cross-coupling reactions prove to be highly efficient for forming new carbon-carbon bonds. In this study, we describe a synthetic strategy for a variety of benzophenone derivatives by activating the carbon-silicon bond of acylsilanes in the presence of a palladium catalyst. Utilizing diaryliodonium salts as coupling partners, which exhibit higher reactivity as electrophiles compared to aryl halides, we successfully synthesized a wide range of functionalized benzophenones with good to excellent yields.

Poster Presentation : **ORGN.P-290**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of α-aminoketone via Photo-Mediated Reactions between Acylsilanes and Imines

Jaewon Lee, Inji Shin*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

α-Aminoketones are important and versatile building blocks in medicinal chemistry, natural products and biologically active compounds. Due to their significance, many efforts have been made to synthesize α-aminoketones. In this study, we introduce a metal-free synthetic method utilizing acylsilanes and imines under photo-irradiation. Visible light activates acylsilanes to form the corresponding siloxycarbene intermediates, which subsequently react with imines to produce α-aminoketones. This approach provides an eco-friendly synthesis of α-aminoketones without the use of transition metal catalyst. After extensive optimizations, functionalized α-aminoketones were successfully synthesized in good to excellent yields.

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Poster Presentation : **ORGN.P-291**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of based-promoted synthesis of isocoumarin derivatives and their synthetic applications

Hee Nam Lim*, Inji Shin[1,*], Serin Hong[1]

Department of Chemistry and Biochemistry, Yeungnam University, Korea

[1] *Department of Fine Chemistry, Seoul National University of Science & Technology, Korea*

We introduce a novel synthetic method for isocoumarin derivatives under mild conditions in the presence of the organic base diisopropylamine (DIPEA). The synthesized isocoumarin derivative, 3-(2-(cyanomethyl)phenyl)-1-oxo-1H-isochromene-4-carbonitrile, exhibits diverse functional groups, suggesting its potential for various structural transformations. Utilizing these isocoumarin compounds, we synthesized several pharmacologically relevant scaffolds through simple transformations. This method offers a promising approach for the efficient synthesis of isocoumarin derivatives with potential applications in pharmaceutical and agricultural chemistry.

Poster Presentation : **ORGN.P-292**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

pH and Redox-Responsive Low-Molecular-Weight Organogelators Based on Quinoxaline Fused Tetrathiafulvalene-Benzoimidazolium Sulfonate

Se young Park, Jung Su Park[*]

Department of Chemistry, Sookmyung Women's University, Korea

Organogel is the type of gel that composed of a gelator and an organic liquid phase within 3D-crosslinked network. Organogels responsive to certain external stimuli including pH, redox, light and temperature have been attracted much attention due to their useful applications, such as sensors, molecular logic gates, and organic electronic materials. As a result, many organogels have been designed, prepared, and developed for various target applications. Among these, designing new building block for multi-stimuli-responsive low-molecular-weight gelators is considered to be highly challenging.Here we represent the synthesis and characterization of zwitterionic quinoxaline fused tetrathiafulvalene-benzoimidazolium sulfonate derivatives. These molecules were fully characterized by NMR spectroscopy, Mass spectrometry, and X-ray crystallography. The optical and electrochemical properties of these molecules were investigated by UV-Vis-NIR, Fluorescence, Cyclic voltammetry, and Differential pulse voltammetry. Interestingly, these zwitterionic derivatives as neutral forms exhibit gelation properties in several organic solvents. Upon changing pH or its redox-state, they undergo gel-sol transition as multi-stimuli-responsive low-molecular-weight gelators. Their morphological properties were also further investigated by Scanning electron microscopy and Dynamic light scattering.

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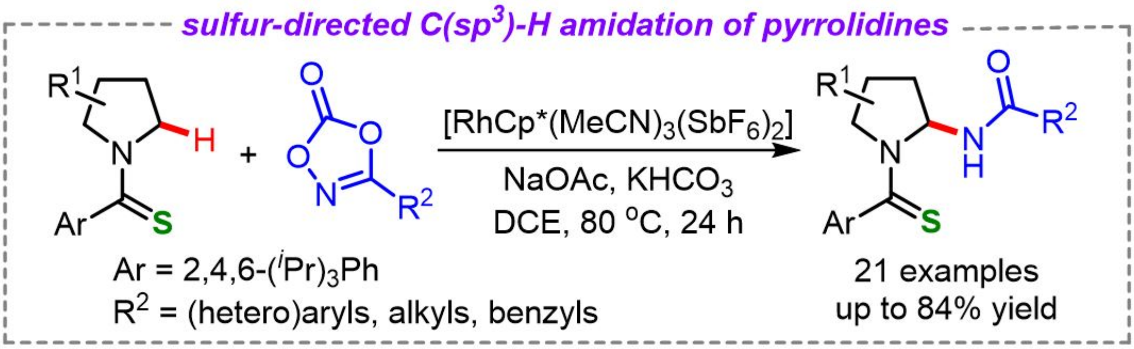
Poster Presentation : **ORGN.P-293**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Rh(III) Catalyzed C(sp^3)−H Amidation of Pyrrolidines via Sulfur-Directing

Jeonghyun Min, In Su Kim[*]

School of Pharmacy, Sungkyunkwan University, Korea

Site-selective functionalization of saturated azacycles such as pyrrolidines is one of central topics in organic synthesis and drug discovery. Although α-amido pyrrolidine derivatives are biologically practical scaffolds, catalytic α-C–N bond formation over α-C–C bond formation of these *N*-heterocycles remains considerably underexplored. We herein report the sulfur-assisted rhodium(III)-catalyzed sp^3 C–H amidation of pyrrolidines with dioxazolones as amidating agents. Dioxazolones are used as robust amidationg sources as the sulfur atom coordinates tightly with transition-metals. The amenability of the thioamide directing group is elucidated by a series of control experiments.



Poster Presentation : **ORGN.P-294**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Micelle-based Supramolecular Cyanine Displacement Assays for Alkyl Ammonium Detection

Goeun Kim, Jung Su Park[1,*]

Chemistry, Sookmyung Women's University, Korea
[1]Department of Chemistry, Sookmyung Women's University, Korea

Amphiphilic surfactant aggregates, called “micelle”, have drawn widespread attention for their utility, used as cleaning agents, catalysts in organic reactions, drug delivery, and even for target analyte sensing. Indicator displacement assays (IDAs) are powerful methods for sensing trace amounts of biologically/environmentally important targeted analytes. Combining two methods, hereby micelle and IDAs, is rarely explored for sensing applications for target analytes. Here we show a series of micelle-based indicator displacement assays (M-IDAs), consisting of benzo-TTF-calix[4]pyrrole (Bz-TTF-C4P), chloride salts of cyanine, and surfactant. These M-IDAs were soluble in water and tested to sense several types of analytes, including alkylammonium, cholines, and nitro-aromatic explosives. Upon adding these analytes to the aqueous solution of M-IDAs, each of the M-IDAs undergoes a change in emission intensity and spectral characteristics depending on the nature of the type of guest species. All these results were further analyzed and rationalized in terms of the binding affinities, quenching efficiency, absorption and emission spectral characteristics of the associated and dissociated chemical species, and type of surfactants.

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Poster Presentation : **ORGN.P-295**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Synthesis and antioxidant effect of aromaticity extended benzimidazole derivatives

Ki wan Park, Jeong Tae Lee*

Chemistry, Hallym University, Korea

Benzimidazole derivatives have physiological activities such as anticancer, antiviral, and antioxidant effect. In addition, Pyrido[1,2-a]benzimidazoles, a derivative of benzimidazole, are known to have fluorescent properties and anticancer and antibacterial effects. Based on these findings, various derivatives of benzimidazole with extended aromaticity were designed and synthesized. All six newly synthesized benzimidazole derivatives were fluorescent. In ABTS assay, all compounds showed almost similar antioxidant effect to vitamin C

Poster Presentation : **ORGN.P-296**

Organic Chemistry

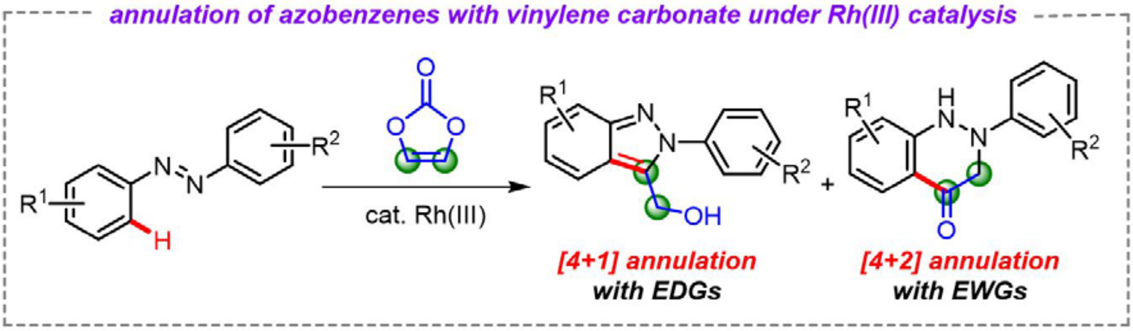
Exhibition Hall 2 FRI 11:00~13:00

Annulation of Azobenzenes with Vinylene Carbonate for Synthesis of (2*H*)-Indazoles and Dihydrocinnolinones via Rh(III)-catalysis

Taeeun Kim, **In Su Kim***

School of Pharmacy, Sungkyunkwan University, Korea

The Rh(III)-catalyzed C−H functionalization and subsequent intramolecular cyclization between azobenzenes and vinylene carbonate is described herein. Depending on the electronic property of azobenzenes, this transformation results in the formation of (2*H*)-indazoles or dihydrocinnolin-4-ones through the generation of *ortho*-alkylated azo-intermediates followed by decarboxylation. Surprisingly, vinylene carbonate acts as an acetaldehyde or acetyl surrogate to enable the [4 + 1] or [4 + 2] annulation reaction. This transformation is characterized by its mild reaction conditions, simplicity, and excellent functional group compatibility.


annulation of azobenzenes with vinylene carbonate under Rh(III) catalysis

Poster Presentation : **ORGN.P-297**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Enhanced Photoswitching Performance of ESIPT-Inspired Dual-Mode Molecules through Resonance Structure Incorporation

Yeju Lee, Juyoung Yoon[1,*]

Chemistry & Nanoscience, Ewha Womans University, Korea

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

In this study, we design and investigate a novel molecular structure aimed at improving the performance of photoswitches based on Excited-State Intramolecular Proton Transfer (ESIPT). Drawing inspiration from ESIPT, we introduce resonance structures to the molecular framework, enhancing the photoswitching capabilities of the designed molecules. The incorporation of resonance structures facilitates fast molecular isomerization in the solid state, contributing to the dual-mode functionality of the photoswitches.The synthesized molecules are systematically characterized, and their photoresponsive properties are compared. Through a comprehensive analysis of each molecule's photoisomerization efficiency, we reveal the impact of resonance structure incorporation on the photoswitching performance. Our findings demonstrate that the introduction of resonance structures leads to improved photoswitching dynamics, making the designed molecules promising candidates for advanced optoelectronic applications. This research not only advances the understanding of ESIPT-based photoswitches but also provides valuable insights for the rational design of high-performance molecular photoswitches with enhanced functionality.

Poster Presentation : **ORGN.P-298**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Converting CO2 into Various Carbonates using Cu(triNHC) catalyst

Changsu Ha, Hye-Young Jang[1,*]

Department of Energy Systems Research, Ajou University, Korea

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

As global warming has become an increasingly pressing issue, interest in the utilization of greenhouse gases, especially carbon dioxide, has increased. In this study, we investigated methods to efficiently utilize CO2 with the Cu(triNHC) catalyst. Through the utilization of the Cu(triNHC) catalyst, we were able to react various epoxides such as epoxy amine, sulfide, and ether with CO2, resulting in the efficient production of carbonates. Through several experiments, it became evident that the characteristics of the Cu(triNHC) catalyst played a crucial role during the reaction, revealing a unique mechanism for carbonate synthesis. These results underscore the potential of the Cu(triNHC) catalyst for CO2 capture.

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Poster Presentation : **ORGN.P-299**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Unified Strategy for Skeleton-divergent Total Syntheses of Monoterpene Indole Alkaloids

Myunghoon Jeong, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Monoterpene indole alkaloids are widely distributed in the natural world, comprising over 2000 members. They exhibit a wide range of biological activities, including anti-cancer, anti-malarial and anti-arrhythmic activities. Despite their structural diversity, they possess intrinsic structural similarity, particularly in terms of the basic skeleton of these natural products. For example, hirsutine, ajmalicine, and yohimbine display a common indoloquinolizidine scaffold with an isopropyl group at C-15 and an ethyl group at C-20 within the scaffold although they possess different basic skeleton.Based on this hidden structural similarity, our group commenced with a research program toward the skeleton-divergent total synthesis of monoterpene indole alkaloids. In this poster presentation, we disclose a skeleton-divergent total syntheses of several monoterpene indole alkaloids bearing a structural similarity. We intend to present the total syntheses of hirsutine, ajmalicine, and yohimbine from a common key intermediate: an indoloquinolizidine bearing an acetyl group at the meta-position of the piperidine D-ring. Through this, we highlight the synthetic strategies employed in the synthesis of these structurally related alkaloids.

Poster Presentation : **ORGN.P-300**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Asymmetric Total Syntheses of 7,8’-Coupled Naphthylisoquinoline Alkaloids

SangWoo Han, Cheol-Hong Cheon[1,*]

department of chemistry, Korea University, Korea

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

Naphthylisoquinoline alkaloids have gained significant attention from the chemistry community due to their structural diversity and promising biological activities. Since the linkage isomers, determined by the coupling positions of two building blocks, can affect their biological activities, the synthesis of these linkage isomers with controlled stereochemistry has attracted considerable attention from the synthetic community. Among the linkage isomers, Of particular interest are the 7,8’-coupled natural products, which exhibit various biological properties such as antimalarial, antiplasmodial, antiparasitic, and antitrypanosomal activities.Despite their interesting biological activities, the synthetic routes to access 7,8’-coupled naphthylisoquinoline alkaloids have been relatively unexplored compared to other linkage isomers. To date, only one total synthesis of 7,8’-naphthylisoquinoline alkaloids with no axial chirality has been reported. Additionally, no efforts have been made to control atroposelectivity in these compounds.Our group has started a research program toward the asymmetric total syntheses of naphthylisoquinoline alkaloids utilizing the central chirality present in the isoquinoline moiety as the atroposelectivity-controlling group. As a continuing our efforts on the asymmetric total synthesis of these alkalodis, we investigated the atroposelective synthesis of 7,8’-coupled naphthylisoquinoline alkaloids.In this poster presentation, we will detail our efforts towards the asymmetric total synthesis of several 7,8’-coupled naphthylisoquinoline alkaloids, exploiting the internal central chirality of the isoquinoline ring to control atroposelectivity.

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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Study on reactivity of Diazoalkanes Generated via [3+2] Cycloaddition of Linear N,N-Disilyl Enamine with Azides

Shinjae Lee, Vinh Do Cao[1], Seewon Joung[1,*]

Department of chemistry, Inha University, Korea

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

We have devised a synthetic approach to produce Z-amidines from cyclic N-silylenamines and organic azides through [3+2] cycloaddition, followed by rearrangement. In the same vein, we utilized borane-catalyzed hydrosilylation conditions to synthesize linear N,N-disilylenamines from conjugated nitriles. These linear N,N-disilylenamines also undergo [3+2] cycloaddition with azides, but the resulting triazoline intermediate follows a different rearrangement pathway, leading to the formation of (E)-form amidine and unstable diazoalkanes as a co-product. To address this unstable diazoalkane, we have developed novel conditions to convert diazoalkanes into esters and pyrazolidines with carboxylic acids and alkenes respectively

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Poster Presentation : **ORGN.P-302**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Discovery of Protease-Activated Receptor 2 Antagonists for Breast Cancer Treatment

Suah Lee, Gyoonhee Han[1,*]

Graduate Program of Industrial Pharmaceutical Science, Yonsei University, Korea
[1]*Department of Biotechnology, Yonsei University, Korea*

Breast cancer is a prevalent and potentially life-threatening illness that impacts a significant number of women on a global scale. Among the elements linked to cell metastasis, protease-activated receptor 2 (PAR2) plays an essential role in impeding the migration and invasion of breast cancer cells. Categorizing breast cancer according to PAR2 expression revealed that individuals with higher PAR2 levels had poorer prognoses. In PAR2-deleted cells, there is a reduction in the activation of downstream signaling, leading to decreased migration and invasion. These findings suggest that suppressing PAR2 could reduce the migration of tissue as a promising strategy for addressing the aggressiveness of breast cancer.Drawing upon prior research utilizing small molecules as PAR2 antagonists, we aim to enhance PAR2 inhibition and improve microsomal stability by optimizing the central structure of the hit compound. We have synthesized eleven compounds thus far as part of this ongoing synthesis process with expectations of identifying an effective PAR2 inhibitor for further enhancement.

Poster Presentation : **ORGN.P-303**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis of C21-C41 Fragment of the Reported Structure of Neaumycin B

Eungyeong Choi, Eunbi Kim[1], Duck-Hyung Lee[*]

Department of Chemistry, Sogang University, Korea

[1]*Chemistry, Sogang University, Korea*

The stereoselective synthesis of the C20-C41 fragment 4 of reported structure of Neaumycin B (1) has been described. C20-C27 fragment 5 was synthesized from commercially available (S)-roche ester using stereoselective allylation, Brown-anti-crotylation as key steps. C28-C41 fragment 6 was constructed from allylic alcohol using Evans-syn-aldol reaction, diastereoselective epoxidation, (S)-CBS reduction as key steps. Finally, boron-mediated aldol reaction led to the of synthesis of C20-C41 fragment 4 of reported structure of Neaumycin B (1).

Poster Presentation : **ORGN.P-304**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Catalytic Potential of Metal-Amyloid Complexes: Exploiting Amyloid Assembly for Supramolecular Catalysis

Seongjae Choi

Applied chemistry, Kyung Hee University, Korea

The assembly resembling amyloid structures not only plays a crucial role in essential biochemical reactions but also exhibits diverse physiological effects in the human body. To harness this phenomenon, we developed a strategy for supramolecular catalysis using self-assembled peptides. This investigation involved the creation of various amyloid fibers through the precise selection of amino acid sequences. Externally aligned functional groups on the surface of the amyloid fibers were exploited to capture metal ions to form metal-amyloid complexes. The structural properties of these complexes were thoroughly examined, along with their involvement in chemical reactions. This research introduces an innovative approach to supramolecular catalysis through metal-amyloid complexes, offering insights that may significantly contribute to exploring the potential applications of these complexes within biological systems.

Poster Presentation : **ORGN.P-305**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Molecular Pringles: Modular Synthesis and Self-Assembly of Saddle-Shaped Aromatics

Myeongsu Jeong, Nam Ki Lee*, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Rigid shapes endow unique mechanical properties to the molecules and assist in the formation of larger structures by self-association. Saddle-shaped molecules, also known as hyperbolic paraboloids, can form stable vertical π-stacked structures through shape complementarity. Here, the pseudo-orthogonal orientation of the four-way flaps around the warped molecular core enhances the mechanical stability of the otherwise weak Van der Waals (vdw) contacts holding an infinite stack. However, synthesizing molecules of hyperbolic paraboloid shape poses significant challenges. To achieve this goal, we have developed triazole-fused cyclooctatetraenes that adopt a saddle shape resembling Pringles chips. These molecules self-assemble into well-ordered 1D π-stacks without the need for strong intermolecular forces such as hydrogen bonding or Coulombic interactions. With appropriate alkyl chains, molecular Pringles rapidly form flexible 1D crystals that can grow up to centimeter length scales and function as waveguides. Moreover, the high modularity of our synthetic design allows for the incorporation of various pendant groups to create a diverse array of functional molecular assemblies. This presentation will discuss the key design principles, synthetic implementations, and current progresses in shape complementarity-driven non-covalent assembly.

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Poster Presentation : **ORGN.P-306**

Organic Chemistry

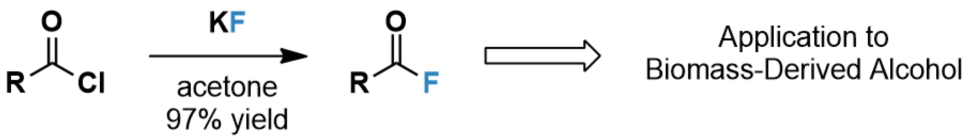
Exhibition Hall 2 FRI 11:00~13:00

Synthesis of Acyl Fluoride via Unusual 1,3-Chelation and Its Application to Chemoselective Acylation of Biomass-Derived Alcohol

Geunho Kim, Jung Woon Yang*

Department of Energy Science, Sungkyunkwan University, Korea

This study presents an innovative and environmentally sustainable approach to synthesizing acyl fluorides, emphasizing their versatility as intermediates in organic synthesis. Unlike other acyl halides, acyl fluorides exhibit exceptional aqueous stability and distinct reactivity, making them invaluable in various chemical transformations.The synthesis of acyl fluoride in this study involves a transhalogenation reaction of acyl chloride with potassium fluoride as a cost-effective fluoride source. A noteworthy aspect of this process is the significant role played by the 1,3-chelation between the K+ ion and acyl chloride, as confirmed by NMR spectroscopy.By utilizing effective 1,3-chelation in the transhalogenation reaction and with the aid of acetone as a factor inducing ion-dipole interactions, the methodology offers a catalyst-free and efficient process for the facile synthesis of acyl fluoride. Furthermore, we successfully applied the synthesis of acyl fluoride to the selective acylation of biomass-derived alcohol.



Scheme 1. Newly designed sustainable chemical process: Acyl fluoride synthesis and its application

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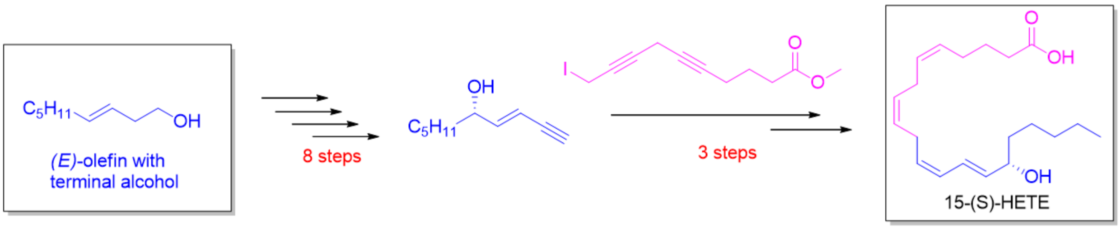
Concise stereoselective synthesis of polyunsaturated fatty acids, 15-(S)-HETE

Myeong su Shin, Youngjoo Byun*

Department of Pharmacy, Korea University Sejong Campus, Korea

Background: 15-S-hydroxyeicosatetraenoic acid (15-(S)-HETE), an endogenous metabolite of 15-lipoxygenase, is known to be a powerful mediator of inflammation. However, the structural modification of 15-(S)-HETE in biological and pharmaceutical applications has not been explored widely. Herein we report the stereoselective synthesis of 15-(S)-HETE. Synthesis: The synthesis of the 15-(S)-HETE commenced by the construction of a chiral alkyne and a propargylic iodide, by a Castro–Stephens coupling, followed by reduction and hydrolysis in overall 97% ee, 38% yield. The synthesis of a chiral aldehyde, a key precursor of the chiral alkyne, was achieved in 34% yield over five synthetic steps. Protection and asymmetric cis-dihydroxylation of the commercially available (E)-olefinic alcohol gave Stereoselective diol in overall 95% ee, 64% yield. The resulting diol was reacted with DMC to afford the chiral vicinal diol-carbonate, which was debenzylated with DDQ and then transformed to the (E)-α,β-unsaturated aldehyde in the IBX-promoted reaction in overall 52% yield. The first fragment, the chiral alkyne, was prepared from the chiral aldehyde by Colvin rearrangement in a three-step sequence and in overall 28% yield. The second fragment, the propargylic iodide, was synthesized in a two-step sequence starting from commercially available reagents. Copper-catalyzed cross-coupling reaction and Appel reaction using NaI delivered the second fragment in overall 32% yield. Conclusion: Stereoselective synthesis of 15-(S)-HETE has been achieved in 3.6% overall yield (ee 97%) 11 steps from commercially available trans-olefin. The corresponding (R)-enantiomer was also obtained in similar ee and synthetic yield.Keywords: Polyunsaturated fatty acids, 15-(S)-HETE, Stereoselective synthesis.


C5H11
OH
(E)-olefin with
terminal alcohol
8 steps
OH
C5H11
I
O
O
3 steps
O
OH
OH
15-(S)-HETE

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Poster Presentation : **ORGN.P-308**

Organic Chemistry

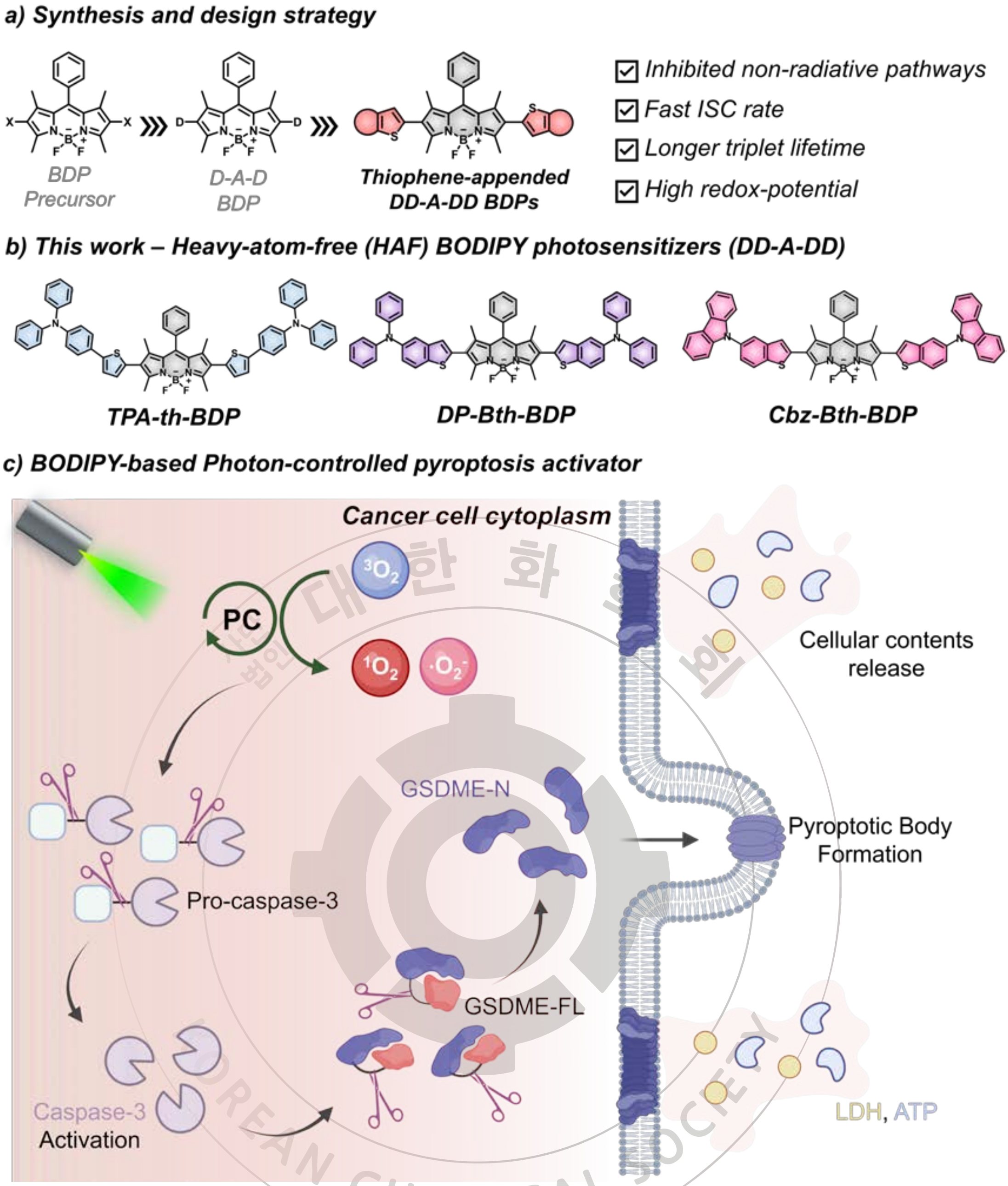
Exhibition Hall 2 FRI 11:00~13:00

Heavy-atom-free BODIPY-based photoredox catalysts as Pyroptosis Inducers

Hyeonji Rha, Jusung An, Jungryun Kim, Qihang Ding, Jaewon Kim, Eunji Kim, Soyu Zi, Yujin Kim, Yunjie Xu, Jong Seung Kim*

Department of Chemistry, Korea University, Korea

Among the strategies attempted as a molecular approach to design efficient BODIPY-based photosensitizers, the conjugation with heavy-atom, e.g. bromine or iodine, at the 2,6-position on BODIPY-based platform provides the longer triplet lifetime that enables to generate reactive oxygen species(ROS). However, halogenated BODIPY photosensitizers potentially lead to dark toxicity, encouraging to design heavy-atom-free ones. Photoexcited BODIPYs generate singlet oxygen via an energy transfer mechanism to oxygens(type-II photosensitization), but have severe limitations in oxygen-insufficient environments, e.g. hypoxic tumors. To address the issues, photocatalytic mechanism in live cells has been emerging in phototherapy. Photocatalytic agents can oxidize biological components such as NADH, crucial bio-molecules for maintaining the metabolism, resulting in disrupting their balance and inducing cellular damage by blocking the tumor’s energy source in mitochondria. Herein, heavy-atom-free BODIPY-based photoredox catalysts(Cbz-Bth-BDP, DP-Bth-BDP, and TPA-th-BDP PCs) were synthesized. These PCs were newly devised to induce cancer cell death by causing a redox imbalance through irreversible oxidation of NADH present in the cancer cell's mitochondria electron transport chain. Cbz-Bth-BDP, carbazole-benzothiophene unit conjugated BODIPY PC, showed more thermodynamically favorable oxidation and reduction potential in a cyclic voltammogram. These results potentiate that Cbz-Bth-BDP efficiently triggers the oxidation of NADH and induces redox imbalances in cancer cells over other PCs. Photo-excited Cbz-Bth-BDP showed the most efficient IC50 value to kill cancer cells and induced the release of LDH, evidence of pyroptotic cell death, working as a photo-induced pyroptotic inducer.



a) Synthesis and design strategy

b) This work – Heavy-atom-free (HAF) BODIPY photosensitizers (DD-A-DD)

c) BODIPY-based Photon-controlled pyroptosis activator

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Organic Chemistry

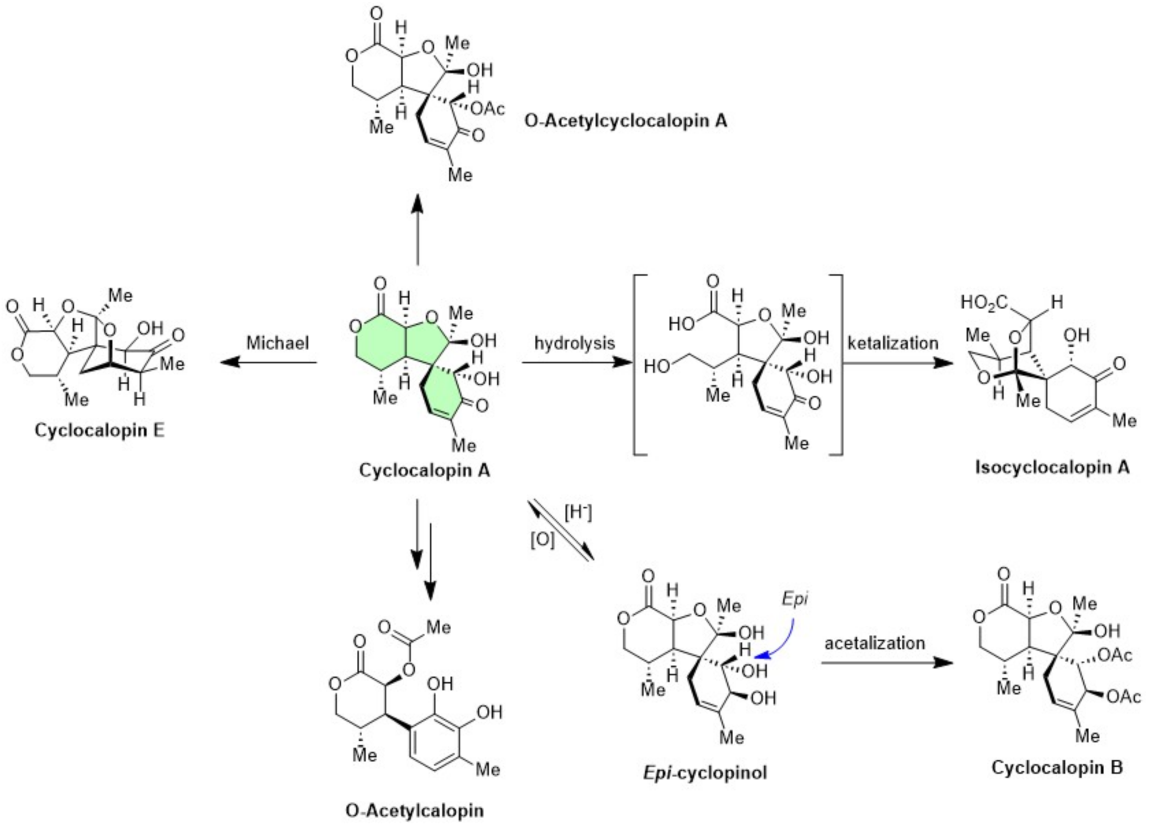
Exhibition Hall 2 FRI 11:00~13:00

Investigation Focused on Building the Tricyclic Core of Cyclocalopin A: Exo-selective Diels-Alder Approach

<u>Jisu Kim</u>, Suh Young Yu, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Mushrooms belong to the category of macrofungi, which yield numerous constituents, including bioactive organic natural products. Within this group, the cyclocalopin family has garnered attention from numerous synthetic chemists owing to its distinctive core structure, comprised of fused and spiro-ring systems. Our goal is to construct the tricyclic core structure of cyclocalopin A, which could serve as a pivotal intermediate for the synthesis of other cyclocalopins through simple transformations. In this presentaion, we will outline significant discoveries made during recent research endeavors focused on synthesizing cyclocalopin A including a cyclocarbonylation and a [4+2]-cycloaddition reaction.


O-Acetylcyclocalopin A
Michael
hydrolysis
ketalization
Cyclocalopin E
Cyclocalopin A
Isocyclocalopin A
[H⁻]
[O]
Epi
acetalization
O-Acetylcalopin
Epi-cyclopinol
Cyclocalopin B

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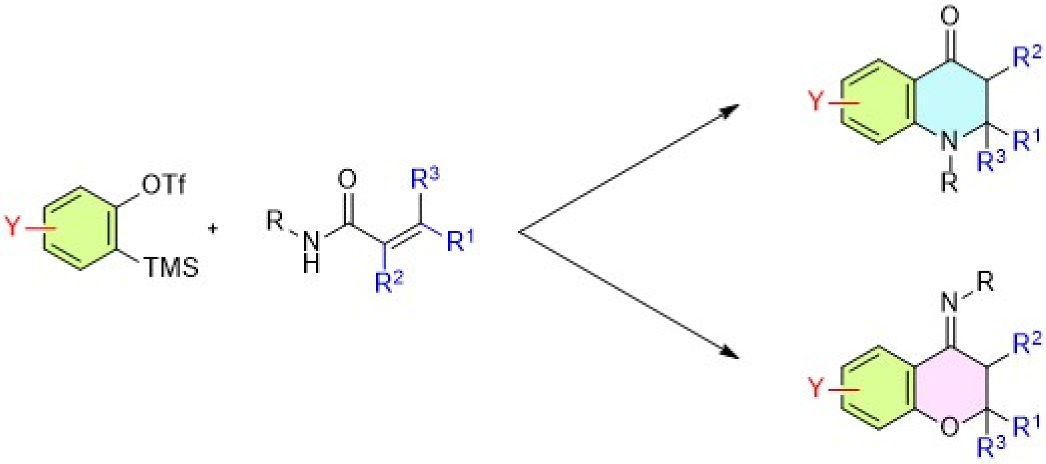
Tandem Aryne Insertion Reaction with Amides

Jihye Lee, Zhang Aimin, Jimin Kim[*]

Department of Chemistry, Chonnam National University, Korea

Aryne species, characterized by their high geometric strain and kinetic reactivity, are esteemed as valuable intermediates in synthetic chemistry for crafting useful chemical architectures. The chemistry of aryne initiates with electrophilic coupling with nucleophiles, facilitated by its bent structure, which results in a lowered LUMO energy level. Herein, we present control factors for a general and efficient method of regulating the regiochemical routes in the reaction from benzyne intermediates. Additionally, we discuss the scope and limitations of this unprecedented transformation, along with mechanistic details elucidating the stereoselectivity.



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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of Enantioenriched Cyclic Allene Precursors Having Various Substituents

Myungsoo Choi, **Sung-Eun Suh**[1,*]

Ajou University, Korea

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

Cyclic allenes, characterized by significant ring strain and unique chirality, are crucial for creating complex three-dimensional molecular structures due to their asymmetric axis and high reactivity. Cyclic allenes as “intermediate species”, being highly reactive and non-isolable and are utilized in the form of functionalized precursors with silyl and triflate groups. These cyclie allene precursors undergo activation via desilylative elimination and in situ participate as the activated forms of cyclic allenes in the reactions with various coupling partners. The previous methods for the preparation of enantioenriched cyclic allene precursors involve the purification step separating their racemic intermediates using a chiral SFC system to obtain their single enantiomers. This study introduces the first method for synthesizing enantioenriched cyclic allene precursors with alkyl and aryl groups that achieves high optical purity through an affordable recyclable chiral auxiliary and eliminates the need for expensive chiral separation systems.

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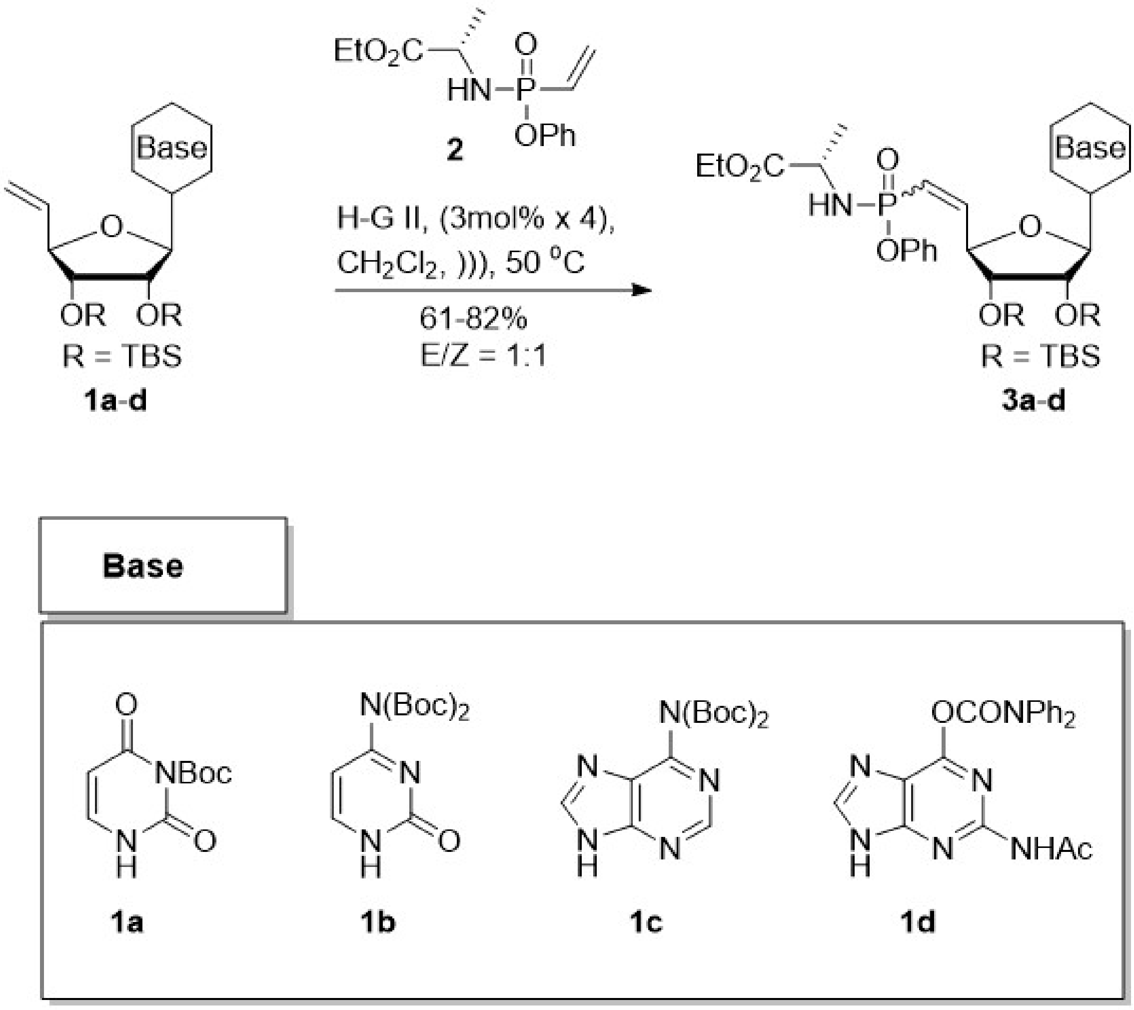
Direct Synthesis of Aryloxy Phosphonamidate Nucleotide Prodrugs Using the Cross Metathesis Assisted by Ultrasonic Irradiation

Se Myeong Choi, Eun Rang Choi, A Young Jung, Jong Hyun Cho[*]

Health science, Dong-A University, Korea

Phosphonate prodrugs, one of mimetic analog of nucleosides monophosphate, have been extensively studied for antiviral nucleoside drug discovery. Currently, the synthetic method of nucleotide phosphoramidate prodrug was well developed by McGuigan that was known as a representative structure of ProTide strategy. However, an efficient strategy for nucleoside phosphonate prodrug is strongly needed on the development of new antiviral agents. Furthermore, there is no approach for direct synthesis of nucleoside phosphonamidate derivatives using the cross metathesis (CM) to date. Herein, we present a direct synthetic strategy of aryloxy phosphonamidate nucleotide prodrugs (A, G, C, and U) was developed with the CM reaction assisted by ultrasonic irradiation and partitioned addition of 12 mol % of Hoveyda−Grubbs (H-G) II catalyst in 61−82% yields as a mixture of *E*-/*Z*-isomers (～2:1) from aryloxy vinylphosponamidate and 5′-vinyl nucleoside moieties.


EtO₂C
HN
P
O
OPh
2
H-G II, (3mol% x 4),
CH₂Cl₂,))), 50 °C
61-82%
E/Z = 1:1
Base
O
OR
OR
R = TBS
1a-d
3a-d
Base
NBoc
N(Boc)₂
OCONPh₂
NHAc
N
H
1a
1b
1c
1d

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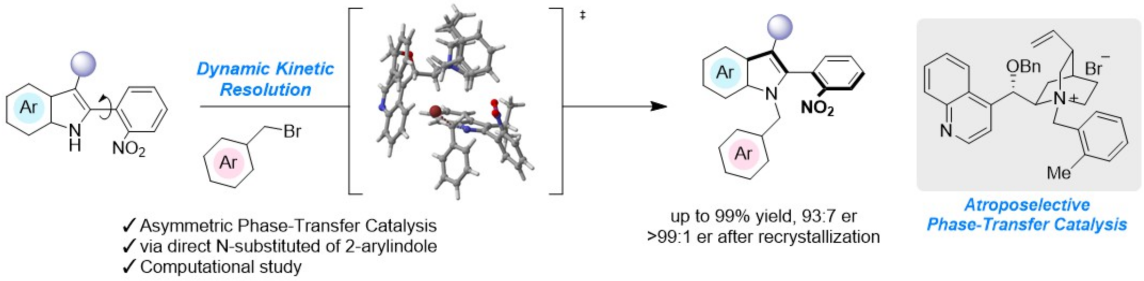
Atroposelective Dynamic Kinetic Resolution of 2-arylindoles by Phase-Transfer Catalysis

Sujin Lee, Yongseok Kwon[1,*]

Sungkyunkwan University, Korea
[1]*School of Pharmacy, Sungkyunkwan University, Korea*

Indoles are a prevalent structural motif found extensively in nature, medicines, and materials with various functions. In particular, 2-arylindoles are acknowledged as a fundamental framework in both natural and synthetic compounds, esteemed for their significant impact on pharmacological effects. However, the investigation of the asymmetric control of the stereogenic axis of 2-arylindoles remains unexplored. Atroposelective substitutions through dynamic kinetic resolution offer potential applications to either the C-3 or N-1 position. While both positions are nucleophilic, the C-3 position undergoes electrophilic aromatic substitution, and the N-1 position favors nucleophilic substitution. To the best of our knowledge, the atroposelective substitution of the N-1 position has not been investigated.This study presents a highly atroposelective dynamic kinetic resolution employing a chiral phase-transfer catalyst. A cinchona-derived catalyst enabled the substitution of 2-arylindoles with benzyl bromide to show excellent enantioselectivieties (up to 93:7 er). We hypothesized that atroposelectivity was achieved by leveraging interactions between the phase-transfer catalyst and the nitro group present in the substrate. Furthermore, we were able to enhance enantioselectivity up to >99:1 er through simple recrystallization. Preliminary computational studies were conducted to gain a more detailed insight into the origins of enantioselectivity. While both transition states benefitted from favorable $\pi-\pi$ interactions between the catalyst and substrate, the undesired enantiomer showed unfavorable steric strain.



✓ Asymmetric Phase-Transfer Catalysis
✓ via direct N-substituted of 2-arylindole
✓ Computational study

up to 99% yield, 93:7 er
>99:1 er after recrystallization

Poster Presentation : **ORGN.P-314**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Ultrasound and H_2O_2 Dual-Responsive Doxorubicin Prodrug

Eunbin Hwang, JunYoung Kim[1], DongHyun Kim[1], Hyo Sung Jung[1,*]

Department of Gerontology(AgeTech-Service Convergence Major), Graduate School of East-West Medical Science, Kyung Hee University, Korea
[1]*Department of Biomedical & Chemical Sciences, Hyupsung University, Korea*

In this study, we report a novel prodrug (DDS-1) with dual reactivity to ultrasound (US) and hydrogen peroxide (H_2O_2) to overcome cardiac toxicity of DOX. DDS-1 is designed with a unimolecular prodrug consisting of boronic ester, lipoic acid, and DOX. The boronic ester moiety within the molecule induces the self-immolative process due to its selective reactivity in the presence of H_2O_2, and the introduction of lipoic acid as another component expects the inhibitory effect of EMT in metastatic cancer. The ability of DDS-1 to drug activity was characterized by UV-vis, FL spectrometer, and HPLC in solution. DDS-1 not only enables efficient DOX release in the presence of H_2O_2 but also demonstrates an increased rate of DOX release and the sono-dynamic therapy (SDT) effect of DOX during ultrasound exposure. These results suggest that the specific activity of DDS-1 in the tumor microenvironment allows for targeted toxicity of DOX to tumor sites and demonstrates the potential for the use of ultrasound to activate small molecule prodrugs as an approach for future clinical applications.

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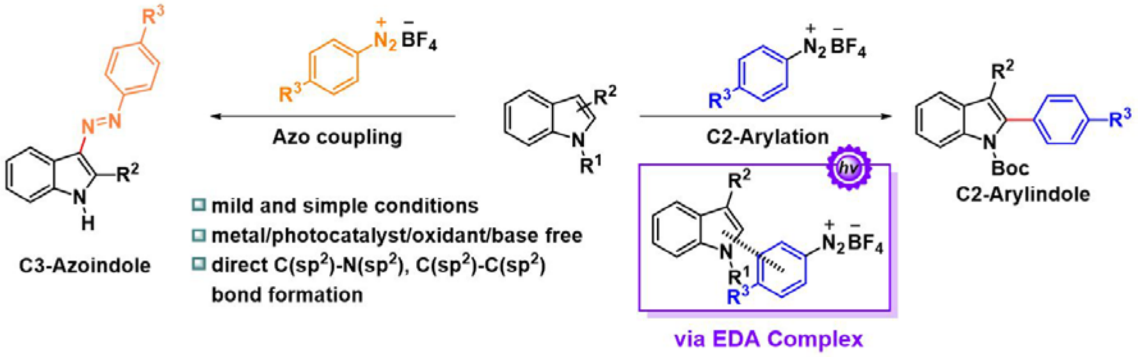
Poster Presentation : **ORGN.P-315**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Chemoselective Arylation and Azo Coupling of Indoles using Aryl Diazonium Salts

Minju Jin, Jeongmin Nam, Eun Joo Kang[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

The biological relevance of the indole scaffold has pushed it to the forefront of synthetic developments.[1] Indoles are representative electron-rich heteroarenes, and the functionalization of indoles has been extensively explored. But there have been no pioneering results on different functionalizations of indole from the same material. We selected aryl diazonium salt as radical source. Aryl diazonium salt is versatile building blocks in organic synthesis, and is well-known as a good free radical source due to its high reduction potential in photoredox chemistry.[2] Herein we report that, reactions for two classes of functionalized indoles via aryl radicals and transformations that retain the dinitrogen group of the aryl diazonium salt. Under relatively mild conditions without an additional metal, photocatalyst, addictive, C2-arylation of N-(Boc)indole and substituted aryl diazonium salts can efficiently occur via electron donor-acceptor (EDA) complex in the presence of visible light. In contrast, under very similar conditions, the reaction of N-H indole exclusively results in azo-coupling in the absence of a light source. Using experimental results, together with density functional theory (DFT) calculations, we found that the reactions can proceed via an electron-donor-acceptor complex.[3] This reaction is an efficient and economically benign synthesis strategy. And azoindole and arylindole products are extremely important because of their good anti-tumor activity in vitro.[4,5]



- mild and simple conditions
- metal/photocatalyst/oxidant/base free
- direct $C(sp^2)$-$N(sp^2)$, $C(sp^2)$-$C(sp^2)$ bond formation

Poster Presentation : **ORGN.P-316**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Ultrasound-triggered Enhanced ROS Generation by a novel BODIPY-Zn complex sonosensitizer

Gihoon Jo, EunGyu Yang, SeongBhin Ahn, Hyo Sung Jung*

Department of Biomedical & Chemical Sciences, Hyupsung University, Korea

Sonodynamic therapy (SDT), utilizing ultrasound (US), stands out as a promising and safe treatment for cancer, with the advantage of enhanced tissue penetration, making it a favorable option when compared to traditional photodynamic therapy (PDT). Nevertheless, the quest for innovative sonosensitizers that exhibit both elevated sonosensitizing efficacy and good biocompatibility poses a formidable challenge. We herein synthesized a novel BODIPY-Zn complex (BSS-Zn) incorporating a hydrophilic short PEG unit and explored its feasibility as a sonosensitizer. BSS-Zn showed enhanced reactive oxygen species (ROS) generation behavior upon US irradiation, surpassing a control sensitizer BSS (an analog lacking the Zn complex) and a commercial sonosensitizer ZnPc (currently undergoing clinical testing, Photocyanine®) in terms of sonosensitizing properties. The increased effect of BSS-Zn was attributed to elevated •OH and O2•− mediated by US irradiation in aqueous media. The SDT effects of BSS-Zn in MDA-MB-231 cells were validated by confirming intracellular types of generated ROS (singlet oxygen (1O2), hydroxyl radicals (•OH), and superoxide (O2•−), respectively) and evaluating cell cytotoxicity in MDA-MB-231 cancer cells. This pioneering research highlights the potential of BSS-Zn as innovative sonosensitizer for SDT. This discovery may open new avenues for the development of more efficient sonosensitizers in the near future.

Poster Presentation : **ORGN.P-317**

Organic Chemistry

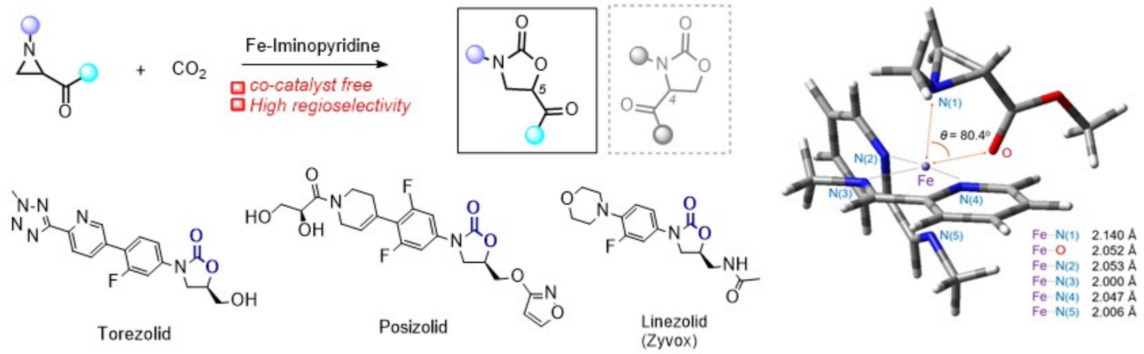
Exhibition Hall 2 FRI 11:00~13:00

Sustainable Fe-Iminopyridine Complexes for the Regioselective Synthesis of Oxazolidinones Using Carbon Dioxide

Junhyeon Choi, Eun Joo Kang*, Jihoon Kim

Department of Applied Chemistry, Kyung Hee University, Korea

Carbon dioxide is an immensely appealing chemical feedstock and a C1 building block due to its widespread availability, low cost, and relatively non-toxic nature. Among the compounds derived from this, cyclic carbamates formed through the cycloaddition reaction of CO2 with aziridines are intriguing chemical substances. Despite the increasing interest in iron catalysts, there has been scarce reporting on sustainable and carbon-balanced approaches to challenging and valuable carbon dioxide conversions using iron-ligand systems. Compared to the CO2 cycloaddition reaction with epoxides, the CO2 cycloaddition reaction with aziridines typically requires harsher conditions. Here, under relatively mild conditions without the need for additional co-catalysts, we can synthesize regioselective 5-oxazolidinones via Fe catalyst1 and aziridine. So far, reactions have only been carried out using aziridines with Phenyl or Alkyl groups2 introduced. Additionally, employing aziridines with an alkyl group results in the formation of 4-alkyl oxazolidinone, while in the case of a phenyl group introduction, 5-phenyl oxazolidinone is formed. In this study, a previously unreported form where carbonyl is substituted in aziridine, and its reaction with CO2 allowed the synthesis of regioselective 5-cabonyl oxazolidinones. Additionally, selectively reducing the carbonyl of oxazolidinones readily forms 5-alkyl oxazolidione, providing an important method for synthesizing building blocks similar to biologically active drugs.


Fe-Iminopyridine
CO$_2$
□ co-catalyst free
□ High regioselectivity
5
4
Torezolid
Posizolid
Linezolid
(Zyvox)
N(1)
N(2)
N(3)
N(4)
N(5)
Fe
O
θ = 80.4°
Fe···N(1) 2.140 Å
Fe···O 2.052 Å
Fe···N(2) 2.053 Å
Fe···N(3) 2.000 Å
Fe···N(4) 2.047 Å
Fe···N(5) 2.006 Å

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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Highly Stereoselective Michael Reactions Catalyzed by Novel Bifunctional Proline Amide-Carboxylic Acid Catalyst

Hyoung Min Yeo[*], **Taek Hyeon Kim**

School of Chemical Engineering, Chonnam National University, Korea

Various aldehydes undergo highly stereoselective Michael reactions with different nitroalkenes in the presence of a novel bifunctional proline amide-carboxylic acid catalyst. This catalyst, easily prepared using commonly available anhydrides and proline linked by a diamine spacer, enables asymmetric catalytic Michael reactions demonstrating high yields (up to 98%), diastereoselectivities (syn/anti, up to 91:9), and enantioselectivity (up to 99% ee) with 5 mol% catalyst and N-methylmorpholine as a base in dichloromethane solvent at room temperature.

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Poster Presentation : **ORGN.P-319**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Mechanochemical Indium(0)-mediated Barbier allylation of Carbonyl Compounds: Unexpected Immiscible Water Additive Effect for Hydrophobic Reagents

Eunsul Go, Nuri Kim, Jeung Gon Kim*

Department of Chemistry, Jeonbuk National University, Korea

Indium-mediated Barbier allylation exhibited a positive effect with the addition of water in mechanochemical ball-milling conditions. A small amount of water as an additive selectively boosted the allylation of solid-state hydrophobic aldehydes despite their immiscibility. Broad scope and scalability of this method are also demonstrated herein.

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Poster Presentation : **ORGN.P-320**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Chemoselective Deoxygenation of N-Heterocyclic *N*-Oxides Using Isopropanol as a Recyclable Reductant

HoKyeong Ryu, YunDo Song, Jun Hee Lee*

Department of Advanced Materials Chemistry, Dongguk University, Korea

The advancement and application of novel synthetic approaches that integrate sustainable reagents and solvents are crucial in both academic and industrial settings. In our ongoing effort to advance synthetic methodologies through visible-light-induced photocatalysis, we were intrigued by the potential of photoredox catalysis to facilitate the removal of oxygen atoms from N-heterocyclic *N*-oxides under mild conditions via single electron transfer pathways. This presentation aims to introduce a novel organic photoredox-based strategy for the chemoselective deoxygenation of diverse functionalized N-heteroaryl *N*-oxides. The catalytic process utilizes isopropanol (IPA) as a reductant and acetone as the solvent. What distinguishes this metal-free protocol is its remarkable capacity to produce easily separable byproducts, specifically acetone and water. Taking advantage of these characteristics, we have successfully conducted gram-scale deoxygenation reactions, eliminating the necessity for expensive and time-consuming column chromatography. Instead, we employ recrystallization and distillation for efficient product separation. Additionally, we showcase the practicality and sustainability of the protocol by demonstrating the efficient recycling of both the reductant and the solvent up to 10 times through a straightforward distillation process. The details of this photochemical protocol, including mechanistic discussion, will be discussed in the poster presentation.

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Poster Presentation : **ORGN.P-321**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

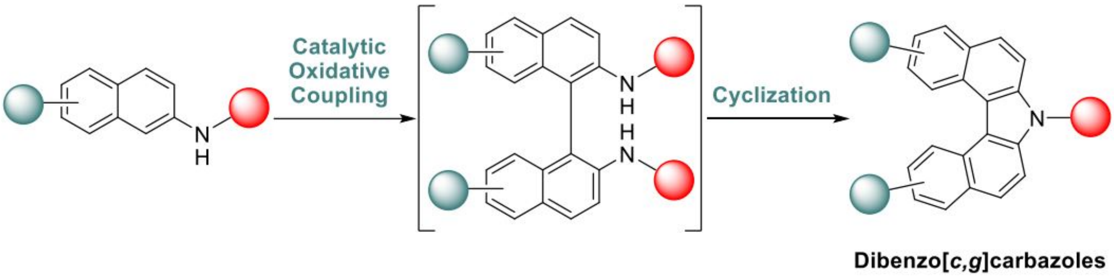
Synthesis of Dibenzo[c,g]carbazole by Copper-catalyed Oxidative Coupling/Cyclization in Tandem Process

Minwoo Kong, **Houng Kang**[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea

[1]*Department of Chemistry Education, Chungbuk Natioanl University, Korea*

In organic material chemistry, chemical compounds with abundant π bonds that undergo hyperconjugation are considered crucial. Specifically, dibenzocarbazole derivatives, among others, have found significance in applications such as organic light-emitting devices and organic electrical devices.1 Various methods have been reported for synthesizing dibenzocarbazole derivatives. For example, the synthesis of dibenzocarbazole through the Buchwald–Hartwig type C-N coupling reaction2 and the Heck-type reaction involving pyrrole and diiodobiphenyl structures.3 However, the necessity of diiodobiaryl has restricted the scope, and the corresponding process has suffered from a lack of functional group tolerance. While the C-H activation method via oxidative coupling is recognized, it utilized an equivalent amount of metal oxide as an oxidant, leading to the generation of numerous metal waste.4 Here, we describe a catalytic approach to construct dibenzo[c,g]carbazoles. A one-pot process featuring copper-catalyzed oxidative coupling and cyclization enables access to various derivatives with diverse functionalities.


Catalytic
Oxidative
Coupling
N
H
Cyclization
N
Dibenzo[*c*,*g*]carbazoles

Poster Presentation : **ORGN.P-322**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

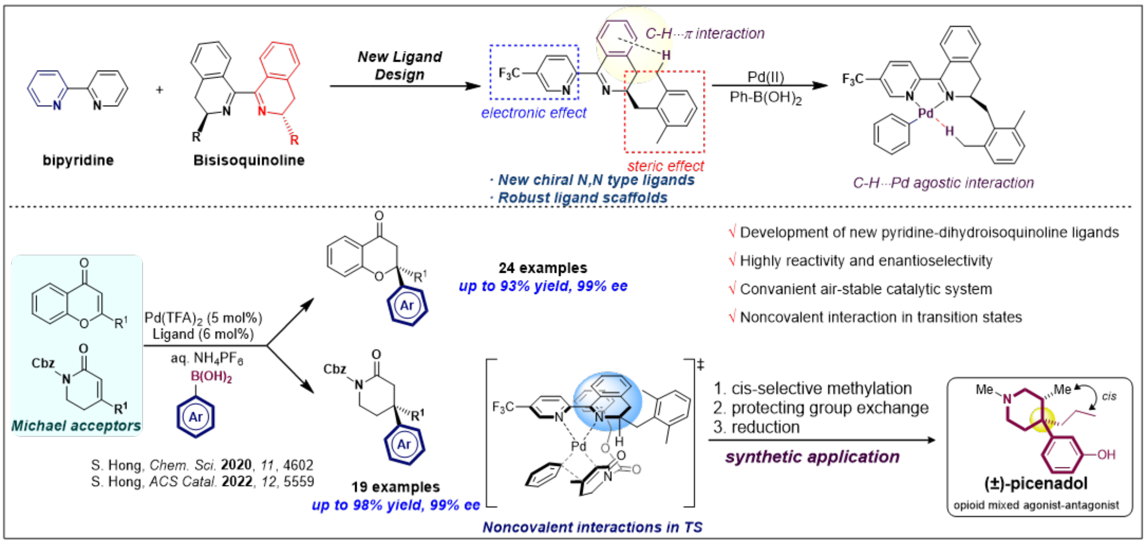
Chiral Pyridine-Dihydroisoquinoline Providing Attractive Noncovalent Interactions

Huijeong Ryu, Sukwon Hong[1,*]

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

[1]*Department of Chemistry, GIST, Korea*

The application of attractive noncovalent interactions has emerged as an elegant strategy in the asymmetric catalysis. Although conventional asymmetric catalysis utilizes repulsive steric interactions to destabilize transition states of minor enantiomers, attractive noncovalent interactions such as ion-pairing, hydrogen bonding, and aromatic interactions could provide an alternative ‘enzyme-like’ pathway to stabilize the transition states of major enantiomers. In our laboratory, Palladium complexes with chiral pyridine-dihydroisoquinoline (PyDHIQ) ligands enabled highly enantioselective conjugate addition reactions of arylboronic acids to 2-substituted chromones and β-methyl α, β-unsaturated δ-lactams. The effect of π- noncovalent interactions on the high enantioselectivity was elucidated by DFT calculations.


bipyridine
Bisisoquinoline
New Ligand Design
electronic effect
C-H···π interaction
steric effect
· New chiral N,N type ligands
· Robust ligand scaffolds
Pd(II)
Ph-B(OH)2
C-H···Pd agostic interaction
Michael acceptors
Pd(TFA)2 (5 mol%)
Ligand (6 mol%)
aq. NH4PF6
B(OH)2
Ar
24 examples
up to 93% yield, 99% ee
19 examples
up to 98% yield, 99% ee
√ Development of new pyridine-dihydroisoquinoline ligands
√ Highly reactivity and enantioselectivity
√ Convanient air-stable catalytic system
√ Noncovalent interaction in transition states
Noncovalent interactions in TS
1. cis-selective methylation
2. protecting group exchange
3. reduction
synthetic application
cis
(±)-picenadol
opioid mixed agonist-antagonist
S. Hong, Chem. Sci. 2020, 11, 4602
S. Hong, ACS Catal. 2022, 12, 5559

Poster Presentation : **ORGN.P-323**

Organic Chemistry

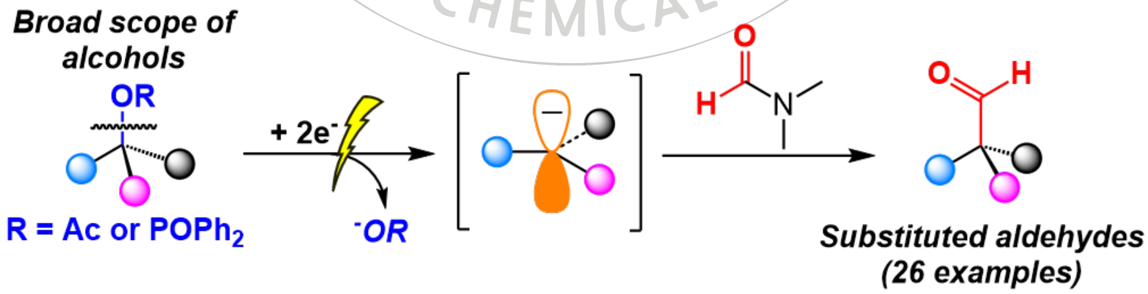
Exhibition Hall 2 FRI 11:00~13:00

Electroreductive formylation of activated alcohols via radical–polar crossover

Jungtaek Kang, Hyunwoo Kim*

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

The direct synthesis of sterically hindered aldehydes is highly challenging. Herein, we report a direct approach to generate such compounds via electroreductive cleavage of the $C(sp^3)$–O bond of activated alcohols. Under the established reaction conditions, benzylic radical intermediates were efficiently generated. A subsequent radical–polar crossover generated carbanions that further reacted with N,N–dimethylformamide to form various aldehydes with tertiary or quaternary benzylic carbon centers. The feasibility of a gram-scale synthesis was also demonstrated. This reaction is also operated in a simple undivided cell, which avoids the use of any transition metal catalysis, toxic gas, and reductants.



Radical-polar crossover via electrochemical reduction

Poster Presentation : **ORGN.P-324**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Regioselective Borobenzylation of Vinyl Arenes by Iron Catalyst

Meng Deyuan, Jaesook Yun[*]

Department of Chemistry, Sungkyunkwan University, Korea

Iron is a ubiquitous metal on Earth and the least toxic metal compared to other transition metals. In recent years, many transition metals have been used for construction of carbon-boron bond, but iron is rarely used in this field. Here, we present a three-component cross-coupling of alkenes, bis(pinacolato)diboron (B2(pin)2), and benzyl tosylates. This iron-catalyzed process facilitates the synthesis of multi-substituted borylalkanes from vinyl arenes and achieves regioselective carbon-boron and carbon-carbon (Csp3–Csp3) bond formation in a one pot process.

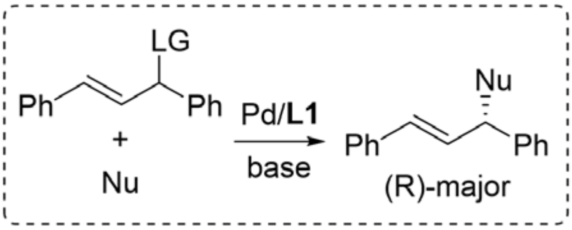
Poster Presentation : **ORGN.P-325**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Origin of Stereoselectivity in Pd-Catalyzed Asymmetric Allylic Substitutions with Trost-Type Mixed Bidentate Phosphorus Ligands

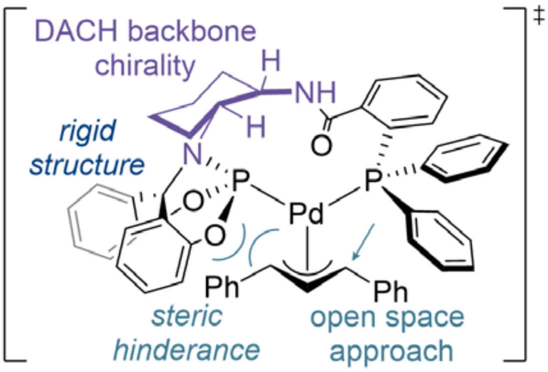
Inkyu Choi, Hyunwoo Kim*

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

In this study, we introduce a novel chiral, unsymmetrical bidentate phosphorus ligand, combining elements from bicyclic bridgehead phosphoramidite and Trost ligand structures, which forms a stable 1:1 complex with palladium without oligomerization, as confirmed by 31P{1H} NMR spectroscopy and X-ray crystallography. This ligand, L1, exhibits exceptional performance in palladium-catalyzed allylic substitution reactions, achieving up to 99% yield and enantioselectivity. Our research includes an analysis of endo- and exo-allyl Pd intermediates, identified by 31P{1H} NMR spectroscopy, and investigates their distinct nucleophilic addition mechanisms. Steric map analysis of these intermediates reveals that the favored transition states involve minimal distortion in the L1Pd-allyl species, leading to high enantioselectivity. This study not only offers a significant advance in ligand design but also enhances the understanding of mechanistic aspects in enantioselective palladium-catalyzed reactions.



- 1:1 complexation with Pd (x-ray structure, ^{31}P NMR)
- ~98% yield
- ~99% ee
- only one possible addition (DFT)



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Poster Presentation : **ORGN.P-326**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Micelle-Based Amplified Fluorescence Turn-on Sensor for Efficient Detection of Trypsin Activity

Minwoo Han, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

In this study, we successfully developed a strategy to monitor trypsin activity using a micelle-based fluorescence and protamine-induced quenching system. We designed and synthesized a pyrene derivative functionalized with four carboxylate to increase its water solubility and enable interaction with protamine (a trypsin substrate) which exhibits a positive charge due to its high content of lysine and arginine. When protamine forms a complex with pyrene derivatives, amplified fluorescence quenching occurs due to exciton migration within pyrene molecules. This complex is decomposed by the enzymatic reaction of trypsin, leading to a sensitive recovery of fluorescence. Based on these strategies, we were able to achieve highly sensitive and selective detection of trypsin, as well as screening of trypsin inhibitors, which are essential for drug discovery.

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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

A Rationally Designed fluorescent Sensor for Selective Detection of Methylmercury in Aqueous Solutions

Haemin Choi, Juyeon Cha, JaeMin Lim, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Among heavy metals, mercury is a highly toxic molecule and poses significant dangers to the environment and health. In the ecosystem, inorganic mercury is easily converted into methyl mercury by microorganisms. Because methyl mercury is fat-soluble, it can easily penetrate the digestive tract and biological membranes, leading to issues such as concentration difficulties, movement disorders, and brain damage. Therefore, we developed fluorescent probe 1 to selectively detect MeHg+ ion. Probe 1 comprises a pyrene moiety combined with a hydrophobic alkyl chain and a boronic acid moiety. Its boronic acid moiety selectively reacted with MeHg+ ions rather than Hg2+ ions, resulting in a change in fluorescence intensity at 348 nm.

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Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Fluorescence Turn-On Sensor for Detecting Mercury (II) ion in Water

Juyeon Cha, Seoung Ho Lee[1,*]

Department of chemistry, Daegu University, Korea

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

Mercury, recognized as a highly toxic heavy metal, is susceptible to environmental pollution in contemporary industrial practices. Upon entry into water, mercury undergoes conversion into highly toxic organic mercury by bacteria and is readily absorbed by living organisms, leading to mercury poisoning. Specifically, mercury accumulation contributes to diseases in the brain, kidneys, and nervous system, underscoring the importance of selectively and highly sensitively detecting mercury ions in water. We employed tetraphenyl ethylene (TPE), which has aggregation-induced emission (AIE) properties, as a fluorophore to establish a "turn-on" system upon aggregation. We also designed the molecule by grafting boronic acid onto it as a recognition site, and incorporating tetraethylene glycol (TEG) to enhance solubility. By detecting mercury ions not only in DI-water but also in tap water and groundwater, we have validated its potential for assessing environmental mecury contamination in various water sources.

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Exhibition Hall 2 FRI 11:00~13:00

A Ratiometric Fluorescent Probe for Detecting Tyrosinase Activity in Human Serum

Minwoo Han, Haemin Choi, Hyeonjeong Seong, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Tyrosinase serves as a significant biomarker for melanoma, a malignant tumor. We have designed and synthesized probe 1 to detect tyrosinase activity, a molecule capable of ratiometric fluorescence measurement employing excited-state proton transfer (ESPT). Probe 1 features a benzothiazole moiety exhibiting ESPT properties, along with a tyrosinase recognition site and a 3-hydroxybenzyl moiety designed to mitigate interference from reactive oxygen species (ROS). Probe 1 exhibits blue fluorescence emission at 418 nm, which shifts to 484 nm upon oxidation of its 3-hydroxyphenyl moiety by tyrosinase through a 1,6-elimination process. Using this ratiometric strategy, we successfully detected tyrosinase activity in human a serum, and screened for tyrosinase inhibitors applicable to skin whitening products and fruit browning prevention.

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Poster Presentation : **ORGN.P-330**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Micelle-based Tturn-on Fluorescent Sensor for Early Diagnosis of Pancreatitis

Haemin Choi, JaeMin Lim, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Acute pancreatitis is a disease characterized by sudden inflammation in the pancreas. Due to the limited symptoms in the early stages, treatment is often delayed. Elevated blood lipase levels are closely associated with pancreatic disease. Therefore, detecting changes in lipase levels is an important method for early diagnosis of pancreatic diseases. Here, we developed a micelle-based fluorescent probe for the quantitative detection of lipase in aqueous solution. When the ester bond of the probe, which is the recognition site of lipase, undergoes hydrolysis, the water solubility of the probe decreases, resulting in induced micelle formation and increased fluorescence. This system represents a sensitive and selective detection method for lipase.

Poster Presentation : **ORGN.P-331**

Organic Chemistry

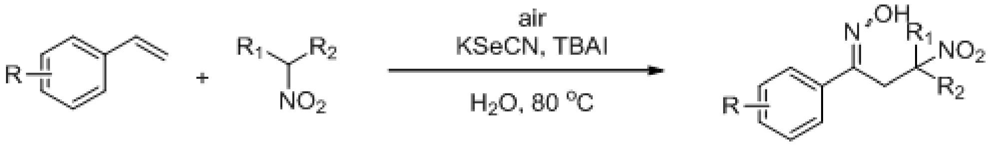
Exhibition Hall 2 FRI 11:00~13:00

Catalytic Aerobic Nitrosation of Styrenes with Secondary Nitroalkane for Oxime Formation

<u>Hyesoo Park</u>, Hun Young Kim*, Kyungsoo Oh*

College of Pharmacy, Chung-Ang University, Korea

Oxime compounds are versatile intermediates widely utilized in organic synthesis. They find applications in the pharmaceutical industry, materials science, and agrochemicals. The traditional methods for synthesizing oximes involve the reaction of hydroxylamine with carbonyl compounds. However, alternative approaches are continually being explored to develop more efficient and environmentally friendly methods for oxime synthesis. Our group recently demonstrated the aerobic N-nitrosation of secondary nitroalkanes in water utilizing a catalytic amount of KSeCN and TBAI. Secondary nitroalkanes underwent the oxygen-induced nitro–nitrite isomerization, highlighting their capability to function as versatile nitrosating agents in aerobic environments. In continuation to our studies, we have developed a facile pathway for the synthesis of oxime compounds by the reaction of substituted styrenes with nitropropanes in good yields (36-86%). The use of water as a solvent in combination with the phase-transfer catalysis system emphasizes the green reaction conditions. This approach presents a promising pathway to oxime synthesis, demonstrating potential applicability across various scientific disciplines.Keywords : Styrene, Nitrosation, Catalysts, Isomerization, Oxime



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Poster Presentation : **ORGN.P-332**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

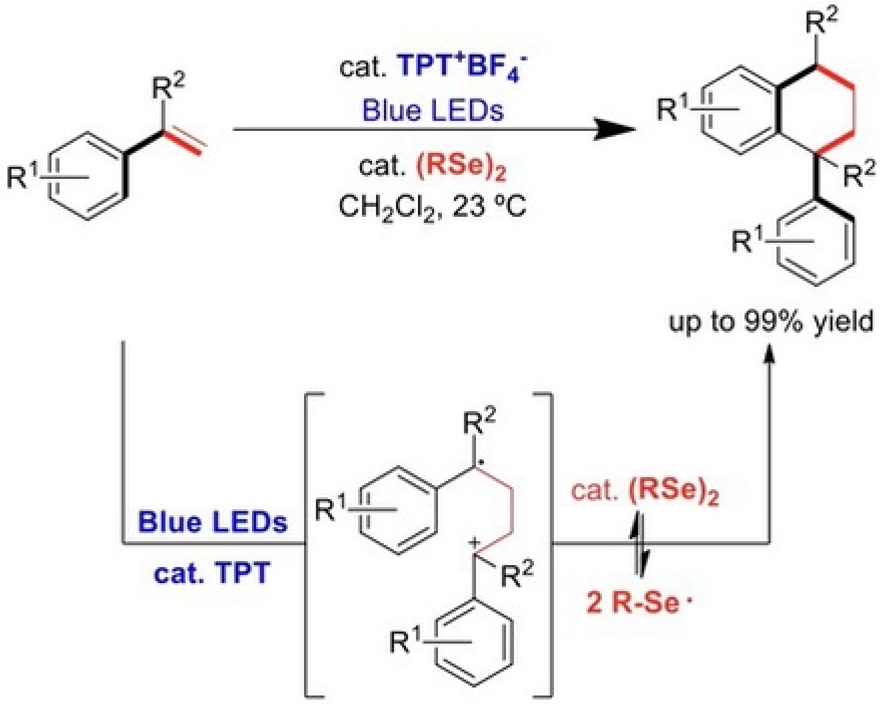
Visible Light [4+2] Homodimerization of Styrenes via Electron Transfer Catalysis of Diaryl Diselenides

Inho Jang, Hun Young Kim[1,*], Kyungsoo Oh[1,*]

Department of Global Innovative Drugs, Chung-Ang University, Korea

[1] College of Pharmacy, Chung-Ang University, Korea

The photochemical activation of styrene derivatives has been suffered from the mixtures of photoadducts derived from the homodimerization via [2+2] and [4+2] cycloaddition pathways in addition to the formation of polymerization products. The uncontrollable electron transfer process of radical cationic intermediate species has been reasoned for the unproductive homodimerization pathways of styrenes. To overcome such unproductive electron transfer processes of radical cation intermediates, we envisioned the highly efficient electron transfer catalysis for the radical cation intermediates to minimize their life-time and energy-wasting back electron transfer processes. In this presentation, a visible-light induced photocatalysis strategy for the [4+2] homodimerization of decomposition-prone styrenes will be introduced, where the diaryl diselenides are utilized as a facile electron transfer catalyst. In this protocol, the [4+2] homodimerization of styrenes was exclusively achieved under the visible-light irradiation, employing $TPT^+BF_4^-$ as photocatalyst and diaryl diselenide as an electron transfer catalyst. Various styrenes exhibiting facile polymerization behaviours smoothly underwent the desired [4+2] homodimerization to give the corresponding tetralin derivatives up to 99% yields. The reaction mechanism will be discussed with spectroscopic data to account for the cooperative roles of photocatalyst and diaryl diselenide under the visible-light irradiation conditions.Keywords : selenium catalyst, radical cation, homodimerization, visible-light


R^2
R^1
cat. TPT$^+$BF$_4^-$
Blue LEDs
cat. (RSe)$_2$
CH$_2$Cl$_2$, 23 ºC
R^2
R^1
R^2
R^1
up to 99% yield
R^2
R^1
Blue LEDs
cat. TPT
+
R^2
R^1
cat. (RSe)$_2$
2 R-Se·

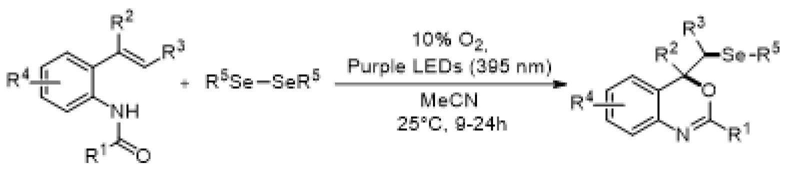
Poster Presentation : **ORGN.P-333**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of Visible Light-Induced Photocatalyst Free Selenocyclization Reactions under Controlled O_2 Atmosphere

Jiwoo Park, Hun Young Kim[1,*], Kyungsoo Oh[1,*]

Department of Global Innovative Drugs, Chung-Ang University, Korea
[1]*College of Pharmacy, Chung-Ang University, Korea*

Organoselenium compounds have attracted great interest due to their pivotal roles in biological redox processes and their synthetic versatilities as intermediates and catalysts in organic synthesis. The electrophilic nature of selenium necessitates the use of catalysts and promoters for selenofunctionalization. In contrast to electrophilic activation strategy, our group previously reported the three-component selenofunctionalization of alkenes with various nucleophiles under visible light irradiation without photocatalyst, where the two selenyl groups in diselenides can be fully utilized through the aerobic oxidation of selenols to diselenides. The key to success was the oxygen content in the reaction medium directing the reaction pathway to the selenofunctionalization products instead of oxidation products. This result prompted us to investigate the oxygen-controlled selenocyclization pathway using an internal nucleophile. In this presentation, visible-light-induced selenocyclizations of *ortho*-vinylanilides will be discussed with the detailed optimization process, substrate scope and reaction mechanism. The 5-10% oxygen concentration was sufficient to induce the homolytic radical scission of diselenides and the redox-neutral selenol oxidation process, effectively supressing the competitive O_2 incorporated oxidation processes. The developed visible light-induced selenocyclization strategy did not require any exogenous photocatalyst and chemical oxidant, only using visible light under low O_2 content. Also, additional developments on selenocyclization will be presented as part of our ongoing research efforts.KeywordsPhotocatalyst-free, Selenocyclization, Visible Light, Aerobic Oxidation, Oxygen-Controlled


R2
R3
R4
NH
R1
O
+ R5Se−SeR5
10% O2,
Purple LEDs (395 nm)
MeCN
25°C, 9-24h
R3
R2
Se-R5
O
R4
N
R1


OH
+ PhSe−SePh
O2
Blue LEDs (470 nm)
MeCN, 25 °C
O
SePh

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Poster Presentation : **ORGN.P-334**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Chromo-fluorogenic rhodamine B-based probe for Cu(II) detection in aqueous solution

Young Woo Noh

Bionano Convergence, Hanyang University, Korea

Copper ions are widely used in different fields of industry and can cause various health issues when exposed to this metal ion. Thus, it is important to regulate and monitor this metal ion in environment and human body. In the current study, we prepared a Cu2+□ sensing probe by connecting an alkyne-functionalized rhodamine B hydrazide to an azide-functionalized ethanol via a copper (I)-catalyzed alkyne-azide cycloaddition (CuAAC) "click" reaction. The resulting probe (1) contains a triazole ring between the rhodamine B and the ethanol units. Upon addition of Cu2+, the probe exhibited intense fluorescence emission at 575 nm (I575) in a binary solvent of acetonitrile:water (1:1 v/v), indicating that the spirolactam ring of the rhodamine B fluorophore opened, induced by the metal ion binding. Upon addition of Cu2+, the probe showed an approximately 20-fold increase in the fluorescence intensity at 575 nm. Importantly, this probe showed high selectivity and minimal interference from other metal ions compared to other rhodamine B hydrazide-derived probes, suggestive of the strong binding between probe 1 and the metal ion. The fluorescence-based limit of detection of this probe was calculated to be 0.13 □M for Cu2+ detection. The molecular interaction of probe 1 with Cu2+ was investigated and elucidated through density functional theory (DFT) and NMR titration methods. The current study demonstrates the potential of a new rhodamine B-based probe (1) for the selective and sensitive detection of Cu2+ in an aqueous environment.

Poster Presentation : **ORGN.P-335**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

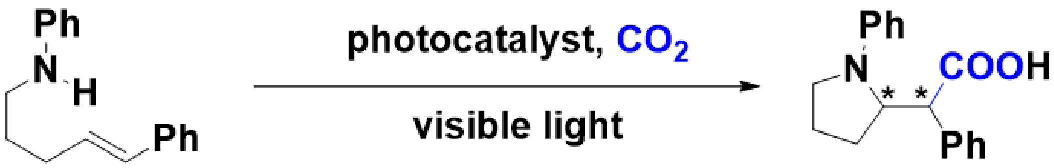
Photo-catalyzed Aminocarboxylation with CO2 for the synthesis of β-Amino Acid

Seungchul Park, Sukwon Hong[1,*]

Gwangju Institute of Science and Technology, Korea

[1]*Department of Chemistry, GIST, Korea*

Utilizing renewable resources is gaining attention as a key element of sustainable development. CO_2 is considered an ideal C1 source because it is sustainable, readily available, and non-toxic. Therefore, transformation of CO_2 into valuable chemicals is highly attractive methods. Carboxylation with CO_2 remains one of the most important topics in this area for upgrading CO_2 to valuable carboxylic acids. Especially, the difunctionalization of alkenes with CO_2 is one of the most useful method for synthesizing various carboxylic acid. To date, many difunctionalization via carboxylation reactions of alkenes and CO_2 have been reported through photocatalysis, transition metal catalysts, and electrochemistry. However, aminocarboxylation has only one example. Yu group reported copper catalyzed aminocaboxylation in photo condition, but it was only able to form β-selective carboxylation products. In this study, aminocarboxylation using α-selective carboxylation has been proposed as a method to form various β-amino acids.



- *photocatalyzed aminocarboxylation with CO_2*

Poster Presentation : **ORGN.P-336**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Photocatalytic Artificial Exoskeletons on Individual Living Cells for Organic-waste Decomposition

Jiwoo Park, Hojae Lee*

Department of Chemistry, Hallym University, Korea

Encapsulation of individual living cells within nanometer-thick, artificial exoskeletons through single-cell nanoencapsulation (SCNE) techniques has provided physicochemical cytoprotection in early-stage technological advancements. Advances in this field demands the development of catalytically active biohybrid systems capable of augmenting the innate biological functions of cells or incorporating abiotic functionalities. Traditionally, cells have been armed with exogenous catalytic capabilities through the integration of enzymes into cytoprotective nanoshells. However, the scope of enzymatic catalysis is confined to specific biochemical reactions tied to cellular metabolism, and enzymes, being sensitive biomolecules, are easily to denaturation under external environmental fluctuations. In this study, we introduce ZIF-8 nanozymes within artificial exoskeletons to endow non-biological photocatalytic properties to cells for the efficient decomposition of organic wastes. ZIF-8, representative metal-organic frameworks (MOFs), exhibits photocatalytic activity under UV-light exposure. Specifically, Saccharomyces cerevisiae cells were initially encapsulated with Fe-trimesic acid (BTC) complexes to prevent UV-induced cell death, followed by the in-situ formation of ZIF-8 layers atop the Fe-BTC layers, thus creating a novel cell@Fe-BTC/ZIF-8 biohybrid system.

Poster Presentation : **ORGN.P-337**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

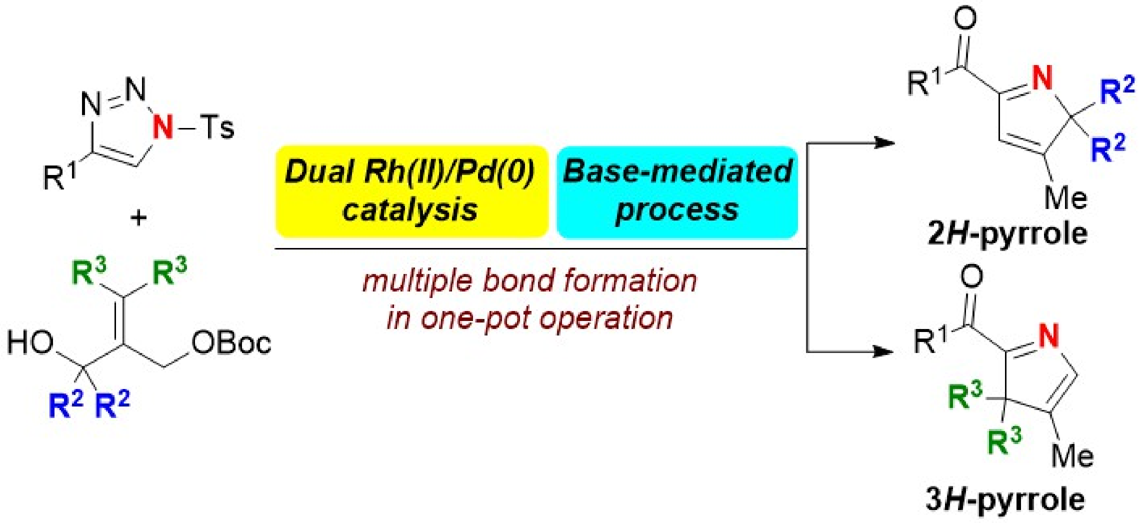
Tandem one-pot synthesis of 2*H*- and 3*H*-pyrrolesenabled by dual Rh(II)/Pd(0) catalysis

Seoung-Mi Choi, Yuri Yun[1], Juhyun Kim*

Department of Chemistry, Dongguk University, Korea

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

2*H*-, and 3*H*-pyrroles are biologically important N-heterocycles found in many natural compounds. However, the synthesis of 2*H*, 3*H*-pyrroles is challenging due to their isomerization. Here, we have developed a successful method for synthesizing 2*H*- and 3*H*-pyrroles have been developed. These methods utilize a combination of dual Rh(II)/Pd(0) relay catalysis and DBU-mediated processes in a one-pot operation, employing N-tosyl triazoles and hydroxymethylallyl carbonates. The synthetic method for 2*H*-, 3*H*-pyrroles utilizes readily available N-tosyl triazoles as stable nitrogen sources of both pyrrole scaffolds, and the regioselectivity of the reaction is controlled by the positions of substituents on the hydroxymethylallyl carbonates.


N=N
N–Ts
R1
+
R3 R3
HO
OBoc
R2 R2
Dual Rh(II)/Pd(0) catalysis
Base-mediated process
multiple bond formation
in one-pot operation
O
R1
N
R2
R2
Me
2H-pyrrole
O
R1
N
R3
R3
Me
3H-pyrrole

Poster Presentation : **ORGN.P-338**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Bisindolizine fluorophore as a new AIEgens

Eunsu Kim, **Eunha Kim**[*]

Department of Molecular Science and Technology, Ajou University, Korea

Traditional fluorophores are typically suffer from quenching upon aggregation, a distinct class of fluorophores exhibits enhanced emission in aggregated or solid-state forms, the phenomenon is termed as ‘aggregation induced emission’(AIE) and the corresponding compound is designated as AIE Luminogen (AIEgen). Indolizine is one of the intrinsically fine-tunable fluorescent skeletons display versatile bioimaging and material applications. In our recent study, we identified an indolizine-based chemical framework with a tunable emission wavelength property, optimized for the synthesis of diverse AIEgens. Owing to the advantage of longer wavelength emission for bioimaging, we envisioned to broaden the emission range of indolizine-based chemical framework beyond the visible range to achieve improved imaging outcomes. Despite of several significant approaches, dimerization approach could be an innovative strategy to tune the fluorophores towards long range emission. In order to support our hypothesis, we have studied the DFT calculation of indolizin-3-yl(phenyl)methanone, the building block for our study. The DFT results are well corroborated with our rationale design of the dimer (bisindolizine). In line with our initial vision, we recognized the importance of establishing a synthetic protocol for our project. Inspired by recent advancements in metal-catalyzed dehydrogenative strategies, we noted that these methods eliminate the need for prefunctionalization of starting materials and target molecules in fewer steps with minimal byproducts compared to conventional coupling reactions. As a result, we envisioned to develop a series of new symmetrical bisindolizine framework as a core skeleton for AIEgen using metal-catalyzed processes. DFT study, detailed synthetic protocol, and photophysical properties of the newly prepared AIEgen will be discussed in the poster presentation.

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Poster Presentation : **ORGN.P-339**

Organic Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Selective protein tagging using Flow Chemistry

Heejoo Shin, Se Won Bae*

Department of Chemistry, Jeju National University, Korea

Tagging fluorescent molecules selectively to proteins has been a continued area of research. In most studies, batch-wise fluorescence tagging has been employed, utilizing a batch process method where all reaction materials are placed into a reaction vessel and allowed to react for a certain period. However, these conventional batch processes suffered from inconsistency in results due to variations in conditions such as temperature and changes in the surface area of reaction materials during the reaction time, leading to difficulties in controlling the yield of reaction products. Furthermore, stability is compromised, and scaling up for commercialization becomes challenging when using batch processes.To overcome these challenges associated with batch processes, we employed flow chemistry. Flow chemistry involves creating reaction products through continuous chemical reactions within flowing fluids. Unlike batch processes, this allows for efficient control of reactions and stable scaling up through automated processes. By controlling the number of fluorescent tags to be attached to proteins based on the residence time of the flow reactor, we were able to achieve consistent results and improve the yield of reaction products through automated processes. Additionally, by using buffers with different pH levels, we were able to find pH values with higher selectivity and efficiency.We have developed a method to selectively tag fluorescent molecules to lysine residues of proteins and control the number of residues reacting with fluorescent molecules through pH and residence time of the flow reactor. The use of automated processes for selective tagging is expected to contribute to the development of the pharmaceutical industry by synthesizing chemical substances other than fluorescent molecules in the future.

Poster Presentation : **ORGN.P-340**

Organic Chemistry

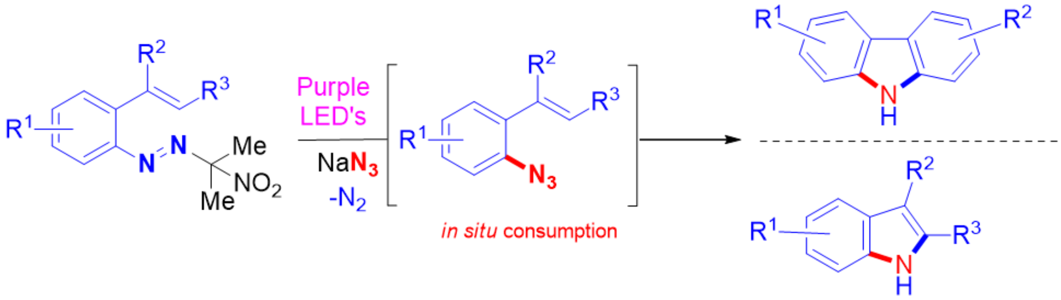
Exhibition Hall 2 FRI 11:00~13:00

Visible Light-Induced Tandem Aromatic S_N1 Reaction-Intramolecular C-H Amination of Areneazo-2-(2-nitro)propanes: One-pot Acess to Carbazoles and Indoles

<u>Rahulkumar Patel</u>, Hun Young Kim*, Kyungsoo Oh*

College of Pharmacy, Chung-Ang University, Korea

Carbazoles and Indole constitutes as an important structural motif in a vast range of natural products, pharmacologically active medications, and materials chemistry. Over the years, to access these compounds various methods have been developed using aryl azides. Nevertheless, the explosive nature of some of the aryl azides disadvantaged the full synthetic potential of aryl azides. In our previous work, we reported areneazo-2-(2-nitro) propane•HCl salts that generate the singlet aryl cation upon visible light excitation, leading to the facile aromatic S_N1 reactions with a variety of nucleophiles. With the improved safety features of neutral areneazo-2-(2-nitro) propane derivatives compared to aryl diazonium salts, our visible light-promoted aromatic S_N1 reactions provide an alternative aryl $C_{sp}{}^2$-X bond forming strategy.In continuous to our previous work, we found that upon visible light irradiation the reaction of areneazo-2-(2-nitro)propanes with sodium azide provided the aryl azides that in situ underwent another visible light photolysis process to give carbazole and indole derivatives. Areneazo-2-(2-nitro)propanes served as a safe alternative of diazonium salts to generate aryl azides for the in situ consumption via photolysis, showcasing the improved safety features of the current method.Keywords: Aryl Cation, Aromatic SN1 Reaction, Visible Light, Aryl Azide


R1
R2
R3
N
N
Me
NO2
Me
Purple LED's
NaN3
-N2
R1
R2
R3
N3
in situ consumption
R1
R2
N
H
R2
R1
R3
N
H

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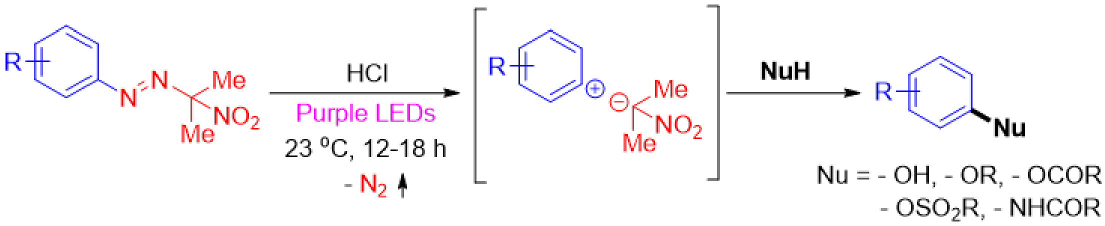
Poster Presentation : **ORGN.P-341**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Visible Light-Induced Aromatic SN1 Reactions of Areneazo-2-(2-nitro)propanes

Dilip vitthal Patil, Hun Young Kim[1,*], Kyungsoo Oh[1,*]

college of pharmacy, Chung-Ang University, Korea
[1]*College of Pharmacy, Chung-Ang University, Korea*

Aryl diazonium salts have been used as precursors in metal-catalyzed and photoredox-catalyzed cross-coupling reactions. The aryl diazonium salts can also generate the aryl cation species under acidic and UV irradiation conditions. However, the free radical chain process and the hydride transfer mechanism do indeed obscure the full synthetic potential of aryl cation intermediates. Moreover, the inherent instability combined with the explosive nature of some aryl diazonium salts are continuously reiterated with safety concerns for industrial application. As safer alternatives to ionic diazonium salts, the aryl diazonium salts with low nucleophilic counterions and the protected form of aryl diazo compounds such as triazenes and azosulfones have been investigated. Nevertheless, the generation of aryl cation species from diazonium alternatives has not been established due to the competing aryl radical generation pathways.Recently, we disclosed our finding on the photochemistry of areneazo-2-(2-nitro) propane•HCl salts that generate the singlet aryl cation upon visible light excitation, leading to the facile aromatic SN1 reactions with a variety of nucleophiles.[1] The in-situ generated singlet aryl cation was stabilized by a bulky counter nitronate anion that prevented other intersystem crossing and single electron transfer processes. With the improved safety features of neutral areneazo-2-(2-nitro) propane derivatives, our visible light-promoted aromatic S_N1 reactions provide an alternative aryl $C_{sp}{}^2$-X bond forming strategy.Reference:1.Patil, D. V.; Karu, R.; Kim, H. Y.; Oh, K. Org. Lett. 2023, 25, 7204-7208.



Scheme 1. Visible-Light-Promoted Aromatic S_N1 Reactions

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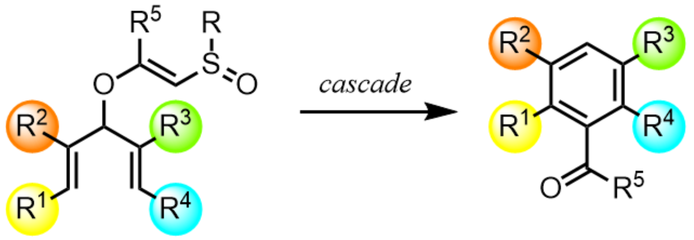
Poster Presentation : **ORGN.P-342**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of a Cascadal Pericyclic Reaction for the Synthesis of Benzene and Nigerapyrone B Synthesis

<u>Heeeun Kim</u>, Yonghoon Kwon[1,*]

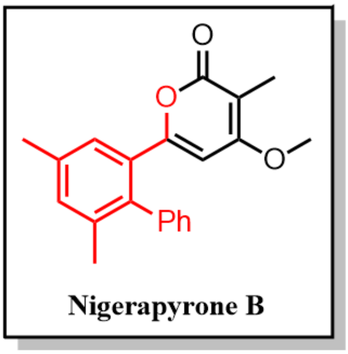
Department of Agricultural Biotechnology, Seoul National University, Korea
[1]*Department of Applied Biology and Chemistry, Seoul National University, Korea*

We developed a novel cascadal methodology to synthesize poly-substituted benzene 2. Easily accessible vinyl ether 1 was transformed into highly substituted benzene 2 through a Claisen rearrangement, sulfoxide elimination, 6π electrocyclization, and auto-oxidation sequence. In this cascade, we can implant the substitution patterns of the divinylcarbinol derivatives into the benzene 2. In addition, depending on the type of R5 substituent, an aldehyde or ketone moiety can be selectively introduced into the benzene ring which is a useful tool for further modifications. Also, we completed the first total synthesis of Nigerapyrone B using the developed method. In this presentation, we provide details on the scope of substrates as well as the characterization of all intermediates.



1

2



Nigerapyrone B

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Poster Presentation : **ORGN.P-343**
Organic Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Substituent Effect on Photochromic Reaction of Benzothiazolinic Spiropyran

Younkyung Cho, Eun Ju Shin[1,*]

Department of Chemistry, Suncheon National University, Korea
[1]*Department of Chemistry, Sunchon National University, Korea*

Photochromic compounds indicate compounds that undergo reversible transformation between colored form and colorless form on the exposure to light. A variety of photochromic compounds have attracted much attention from many research groups due to their wide application to chemical sensors, optical devices, and many other fields. Since first discovery in the early 20th century, a variety of spiropyran derivatives has been extensively studied as typical photochromic compounds, whose molecular structure can be interconverted by UV light irradiation. Their photochromism was discovered in 1952, due to their versatile application in diverse fields. They would undergo reversible structural transformation between a colorless ring-closed spiropyran(SP) form and a colored ring-opened merocyanine(MC) form upon light, temperature, pH, metal ions, chemical species, or mechanical forces, which has been shown to exhibit extremely sensitive absorption and color changes in the visible range. In particular, metal cation driven photochromic transformation of spiropyran has been received wide attention, because various metals, especially transition metals and heavy metals, play important roles in biological, environmental, material, and industrial fields. There are much less studies on benzothiazolinic spiropyrans in comparison to spiropyran. In this study, spiropyran derivatives containing benzothiazoline were synthesized and characterized. Based on the absorption and fluorescence spectra, it is interesting to investigate how the presence or absence of sulfur in spiropyran affects its photochromic properties. Additionally, the substituent effect on the photochromic reaction of benzothiazolinic spiropyran will be studied.

Poster Presentation : **MEDI.P-344**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Study on the inhibitory effect of BuChE using lipoic acid-tryptamine derivatives

Da yeon Song, Min Kyung Shin, Dabin Jeong, Jeong Ho Park*

Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea

In this study, four amide derivatives were synthesized using lipoic acid and tryptamine or 5-methoxy tryptamine directly or using a triazole linker through a click reaction. The inhibitory effect on BuChE was measured using four derivatives, and the correlation between the inhibitory effect and the molecular model was analyzed through computer modeling. The IC50 values of the derivatives in which tryptamine and 5-methoxy tryptamine were directly linked to lipoic acid or the derivatives in which 5-methoxy tryptamine and lipoic acid were linked through a triazole linker were similar (around 28 uM). However, the IC50 value of the derivative in which tryptamine and lipoic acid were linked by a triazole linker was 0.42±0.29 uM, which was more than 60 times better than that of other derivatives. In molecular modeling, the binding energy of this compound was -9.138 kcal/mol, which was higher than that of other compounds. A hybrid compound synthesized from two natural product derivatives using an appropriate linker had selective inhibitory activity against BuChE. (The four compounds did not show inhibitory activity against AchE)

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Poster Presentation : **MEDI.P-345**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

In silico high throughput virtual screening for the identification of dual-target modulators

Soo Won Lee, Juyong Lee[1,*]

College of pharmacy Seoul National University, Korea

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

This study utilizes docking calculations and deep learning models to swiftly identify molecules within a large database that can simultaneously regulate the activation and deactivation of two proteins. The aim is to discover compounds that effectively bind to both target proteins, thereby controlling a specific biological reaction. Through this process, five molecules have been identified and are currently being tested in in vivo experiments.

Poster Presentation : **MEDI.P-346**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Design and synthesis of Sirt6 activator for pancreatic cancer

Noh Gyoungho, Duyeon Choi[1], Hwang Hyeongseop[2], Do Hyun Ryu, Hee Jung Jung[2,*]

Department of Chemistry, Sungkyunkwan University, Korea

[1]*Department of pharmacy, Chungbuk Natioanl University, Korea*

[2]*Center for Rare Disease Therapeutic Technology, Korea Research Institute of Chemical Technology, Korea*

Sirt6 is a mammalian protein and a member of the sirtuin family with deacetylase activity. Sirt6 acts as a tumor suppressor that inhibits the transcriptional activity of c-MYC by deacetylating histone protein. Decreased Sirt6 has been observed as a poor prognosis for several cancers, among which pancreatic ductal adenocarcinoma has been identified as an example. To develop a novel Sirt6 activator (4), which was prepared in two steps. (2) was obtained by iodination (1), which was reacted with N-iodosuccinimide. (3) was obtained by Suzuki Coupling, which was reacted with boronic acid compound. (4) was obtained by Ullman reaction, which was reacted with cooper iodide, aromatic compound. Many compounds were obtained through the last synthesis, and several compounds showed good activity at 10μM.

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Poster Presentation : **MEDI.P-347**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis and biological activities of TLR-modulating compounds and ENPP-1 inhibitors

Eun hyo Lee, Eun Joo Roh[1,*]

Department of Biotechnology, Korea University, Korea

[1]*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

I. TLRs (Toll-like receptors), a subset of PRRs (Pattern Recognition Receptors), detect pathogen-specific molecular patterns, initiating immune responses. TLR3/7/8 respond to viral RNA, and TLR9 detects unmethylated CPG DNA sequences from bacteria. TLR activation regulates immune responses via transcription factors like NF-κB and IRF. Utilizing TLR3/8/9 activation can enhance vaccine efficacy, while inhibiting TLR pathways can improve immune anti-cancer effects. These strategies are vital for strengthening immune responses across diverse tissues.II. Inhibiting ENPP1 (Ectonucleotide pyrophosphatase/phosphodiesterase-1) shows potential therapeutic effects for enhancing immune responses in "cold" tumors resistant to current checkpoint inhibitors. The cGAS-STING pathway, crucial for innate immunity, detects cytosolic DNA, triggering immune activation. However, ENPP1 dampens this response by degrading cGAMP. Targeting ENPP1 could amplify immune reactions, making it a valuable target for cancer immunotherapy research.Our study aims to synthesis and evaluate compounds capable of modulating the functions of both targets, TLRs and ENPP1, which are critical in regulating immune responses. By targeting these pathways, the research aims to enhance immune reactions, potentially advancing cancer immunotherapy.

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Poster Presentation : **MEDI.P-348**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

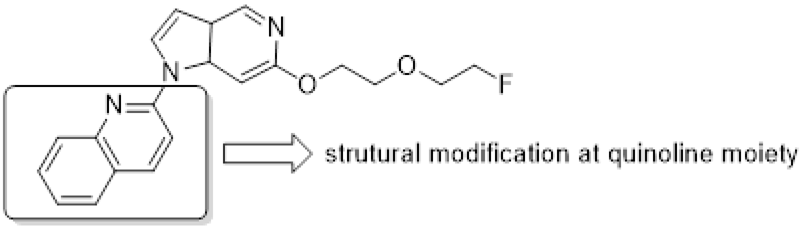
Synthesis of Azaindole derivative with a modified structure in the quinoline moiety as PET imaging probe for tau protein.

Siwoo Lee, Dong Wook Kim[1,*], Su Yun Lee[1]

Molecular imaging chemistry lab, Inha University, Korea

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

Alzheimer's disease, which causes dementia, is known to be caused by the formation of neurofibrillary tangles (NFT) through hyperphosphorylated tau, disrupting neuronal function. Therefore, the development of these tau tracers is essential for accurate diagnosis and early detection of AD. In recent studies, it has been revealed that quinolinyl azaindole derivatives such as KR201,MK-6240 exhibit a high binding affinity for tau proteins. Taking inspiration from this, our research team created derivatives based on MK-6240 and KR201. In the previous study, Our derivative was synthesized from 6-methoxy-1H-pyrrolo[3,2-c]pyridine and 2-chloroquinoline. The introduction of an oligoethylene glycol chain into the azaindole moiety of the lead compound resulted in superior biological test and PET study. In this study, we maintained the structure of the existing 5-azaindole group and synthesized new Azaindole derivatives by modifying the structure in the quinoline moiety. A total of 17 derivatives with modified quinoline moieties were created. In vivo and in vitro tests are performed with these synthesized substances to confirm the appropriate biocompatibility characteristics.



5-azaindole 6-position derivatives

Poster Presentation : **MEDI.P-349**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

A Lipid Nanoparticle Platform Incorporating Trehalose Glycolipid for Exceptional mRNA Vaccine Safety

Soyeon Yoo, Gyo chang Keum*, Eun-Kyoung Bang*

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

The rapid development of messenger RNA (mRNA) vaccines formulated with lipid nanoparticles (LNPs) has contributed to the control of the COVID-19 pandemic. However, mRNA vaccines have raised concerns about their potential toxicity and clinical safety, including side effects, such as myocarditis, anaphylaxis, and pericarditis. In this study, we investigated the potential of LNP-containing trehalose glycolipids (LNP126) to reduce the risks associated with ionizable lipids. Trehalose glycolipids can form hydrogen bonds with polar biomolecules, forming a stable LNP structure by replacing half of the ionizable lipids. The efficacy and safety of LNP126 were evaluated by encapsulating the mRNA encoding the luciferase reporter gene and measuring gene expression and organ toxicity, respectively. Furthermore, mice immunized with an LNP126-formulated mRNA vaccine expressing influenza hemagglutinin exhibited a significant reduction in organ toxicity, including in the heart, spleen, and liver, while sustaining gene expression and immune efficiency, compared to conventional LNPs (Con-LNPs). Our findings suggest that LNP126, a trehalose-based LNP, could facilitate the development of safe mRNA vaccines with improved clinical safety.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **MEDI.P-350**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Radiosynthesis and evaluation of ^{68}Ga labeled chlorinated benzamide derivative for detection of melanoma in small animals

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Malignant melanoma can be removed with surgical techniques in the early stages. However, new technologies are needed to detect malignant melanoma at an early stage because the mortality rate increases dramatically after the occurrence of metastasis. The benzamide structure is known for targeting melanin, which is a specific biomarker of melanoma, so we developed a new chlorinated structure based on benzamide structures. Structural analysis was performed by liquid chromatography-mass spectrometry (LC-MS). The radiochemical yield and radiochemical purity of the ^{68}Ga chelated complex were confirmed by radio thin layer chromatography. *In vitro* uptake was measured in the B16F10 (mouse melanoma) cell line, and in vivo studies were performed with B16F10-bearing mice. The radiometal ^{68}Ga was chelated with the non-decay-corrected radiochemical yield of 61.5% at 95℃ for 10 minutes at pH 5, and the radiochemical purity exceeded 94%. Cell uptake of labeled compound was was significantly higher in melanin-expressing cells than in non-melanin-expressing cells. Furthermore, this compound successfully imaged B16F10 xenografts using microPET in small animals. A new chlorinated benzamide derivatives successfully chelated ^{68}Ga and specifically targets melanin. In addition, MicroPET results showed that the compound provides good visualization of melanin-expressing tumors. Therefore, this structure may have potential as an imaging agent for malignant melanoma with melanin overexpression.

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Poster Presentation : **MEDI.P-351**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

^{68}Ga labeled iodinated benzamide derivative: synthesis and evaluation as a PET imaging agent for malignant melanoma

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Malignant melanoma has one of the highest mortality rates of any cancer because of its aggressive nature and high metastatic potential. The benzamide-based derivatives are known for effectively binding to melanin in melanoma within the current broad spectrum of studies. Based on these research findings, we synthesized the ^{68}Ga-labelled 2,2',2",2"'-(2-(4-(3-(2-((2-(5-iodopicolinamido)ethyl)(methyl)amino)ethyl)thioureido)benzyl)-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrayl)tetraacetic acid, which involves the halogen element I for the detection of melanoma using positron emission tomography (PET). We synthesized the precursor using 5-iodopicolinic acid, 2,2'-diamino-N-methyldiethylamine, and (p-SCN-Bn)-DOTA. After labeling the precursor with ^{68}Ga in a reaction vial at 95°C and pH 5 for 10 minutes, the radiochemical purity of the ^{68}Ga labeled compound was assessed using radio thin-layer chromatography. Cellular uptake of iodinated benzamide derivative was measured in B16F10 cell line (mouse melanoma) after treatment of L-tyrosine. MicroPET studies were performed at 30 and 60 minutes after intravenous injection of the labeled complex into the B16F10 bearing mice.The non–decay-corrected radiochemical yield was 65.8%, and the radiochemical purity exceeded 98%. ^{68}Ga labeled compound exhibited higher cell uptake in melanin-expressing B16F10 cells than in melanin non-expressing cells. Furthermore, this compound successfully demonstrated imaging of melanoma in B16F10-bearing mice through PET. The following results revealed that ^{68}Ga labeled iodinated benzamide derivative has the potential for melanoma diagnosis.

Poster Presentation : **MEDI.P-352**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis and evaluation of brominated benzamide derivative for melanoma detection using positron emission tomography

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Malignant melanoma has the highest mortality rate of any skin cancer due to its aggressive nature and high potential for metastasis. Therefore, early diagnosis and treatment are critical to improving outcomes for melanoma patients. We synthesized a brominated benzamide derivative, 2,2',2",2"'-(2-(4-(3-(2-((2-(5-bromopicolinamidoethyl)(methylamino)ethyl) thioureido)benzyl)-1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrayl) tetraacetic acid, labeled with the radioisotope ^{68}Ga and evaluated biological properties as an imaging agent for melanoma detection using positron emission tomography (PET). To label the synthesized precursor with ^{68}Ga, the eluted ^{68}Ga was dissolved in 0.1 M NaOAc buffer (pH 5.5) and chelation was carried out at 95°C for 10 minutes. The radiochemical yield and radiochemical purity of the ^{68}Ga chelation complex were confirmed by radio thin-layer chromatography (radioTLC). In vitro uptake was measured in the B16F10 (mouse melanoma) cell line, and in vivo studies were performed with B16F10-bearing mice.The radiometal ^{68}Ga was chelated with a radiochemical yield of 76% at 95°C for 10 minutes at pH 5, and the radiochemical purity exceeded 98%. The compound labeled with ^{68}Ga showed high uptake in B16F10 cells expressing melanin The labeled compound could allow visualization of B16F10 xenografts on microPET after intravenous injection for 60 min.The newly developed brominated compound successfully chelated the radiometal ^{68}Ga. This labeled compound has efficacy as a diagnostic agent for malignant melanoma diagnosis. Moreover, if therapeutic radiometals replace diagnostic radiometals, they can potentially be used as therapeutic agents for malignant melanoma treatment.

Poster Presentation : **MEDI.P-353**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Investigation study of Organelle-Targeted Fluorescent Sensor Structure Activity Relationship for Optimal Membrane Binding and Transfer of Lipid Imaging Agents.

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Fluorescent dyes are a versatile class of chromophore. Cyanine has been shown to stack on the end of double-stranded DNA, like a terminal base pair. In all of these cases, changes in the fluorescence efficiency of the dye due to sequence-specific interactions with the labelled strand of DNA or RNA may introduce biases into measurements. The NIR window lies between about 500 and 800 nm, and it is an important criterion to design dyes within this wavelength range for in vivo imaging. Their optical properties including molar absorptivity, fluorescence, and quantum yield, were measured as well as their hydrophobic effects in polar buffer solution. Mitochondrial target specificity is demonstrated by colocalization experiments using the mitochondrion-tracking probes. We envision that cancer cell mitochondrial incorporation of the positive charged cyanine dyes are expected to depolarize mitochondrial membrane potential. Therefore, its effect on malignant mitochondrial targeting, incorporation, staining, membrane potential depolarization, and multicolour imaging application is investigated using human carcinoma cell lines. Along with a long-term plan to develop optical sensors for pH measurements in various biomedical samples, we choose to investigate lipid-anchored conjugates of pH-responsive cyanine dyes (Cy3, Cy5, Cy7) because, these dyes are fluorescent compounds, and their deep red absorption/emission bands are well-suited for biological imaging. Based up on the above evidences, we aim to designed a cancer-targeting cyanine-cholesterol by using different easily cleavable linkers as a carrier to deliver therapeutic agents, with each successive modification to increase hydrophobicity, which appear to be an attractive approach.

Poster Presentation : **MEDI.P-354**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of Novel Cell-permeable Macrocyclic Peptide Inhibitors for Oncological Target MAGE-A4

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Cancer Testes Antigens (CTAs) are a group of proteins with restricted expression in male germ cells in the testis. The immunogenicity and tumor-restricted expression of CTAs make them promising cancer therapy targets. One important family of CTAs is the Melanoma-associated antigens (MAGEs). Recent research by Dr. Cyrus Vaziri has shown that MAGE-A4 is a stabilizing factor for RAD18, which is an E3 ubiquitin ligase that activates the proliferating cell nuclear antigen (PCNA) via monoubiquitination, followed by the TLS pathway activation. Depletion of MAGE-A4 in MAGE-A4-expressing cancer cells destabilizes RAD18, leading to failure to resume DNA synthesis. The mechanism by which MAGE-A4 stabilizes RAD18 is not yet fully understood; however, targeting the MAGE-A4–RAD18 signaling axis can be a promising therapeutic strategy for treating chemo-resistant carcinogenesis due to its selective potential to sensitize cancer cells to intrinsic and therapy-induced DNA damage while having no adverse effects on normal cells.Recently, we have identified a cyclic macro peptide called MTP-1 that selectively binds to MAGE-A4 and disrupts its interaction with RAD18 by targeting the binding domain, also known as the MAGE homology domain (MHD). However, poor cell permeability hinders its effect on regulating the TLS pathway in DNA damage-tolerant cells, highlighting the need for more cell-permeable compounds to interrogate the role of MAGE-A4:RAD18 in the TLS pathway. Therefore, here we intend to optimize the current hit peptide through medicinal chemistry and structure-based design to develop selective, potent, and cell-permeable chemical probes to ameliorate chemoresistance in cancer cells and establish MAGE-A4 as a druggable target for selective cancer therapy.

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Poster Presentation : **MEDI.P-355**
Medicinal Chemistry
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Exploring the Influence of Water on Collagen Triple Helix Stability

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Collagen is an essential protein that offers structural support to diverse body tissues through its unique triple helix structure composed of repeating XYG triplets. Collagen stability is vital for proper tissue function and any disruptions in its stability can lead to various health problems. While previous investigations have revealed various factors influencing collagen stability such as peptide composition, temperature, pressure and pH; the role of water remains insufficiently understood despite its fundamental presence in biological systems. In this study, we employed molecular dynamics simulations to investigate the dynamic interactions between collagen triple helix and surrounding water molecules at the atomic level. We performed simulations on collagen model peptides exhibiting varying stability [(GPO)7, (POG)7 and (OGP)7] and observed differences in their hydrogen bonding with surrounding water molecules, as well as in the water networks surrounding these peptides. Our findings reveal that water molecules engage in intricate hydrogen bonding with collagen residues and organize into topological water networks (TWNs) around collagen chains. This process is crucial for maintaining the structural stability of the collagen triple helix. Our results provide novel insights into the contribution of water molecules in preserving the collagen stability.

Poster Presentation : **MEDI.P-356**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Discovery of Azaindole and Azapaullone as Potent and Selective CDK9 Inhibitors

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7-Azaindole is a highly attractive core as a kinase inhibitor due to its ability to form hydrogen bonds with the hinge of the kinase through its two nitrogens. These azaindole derivatives have shown kinase inhibitory activities in kinase such as BRAF, JAK3, and CDK. Among them, Cyclin dependent kinase (CDK) forms a complex with cyclins and regulates cellular functions such as DNA replication, transcription, and apoptosis. Specifically, CDK9 complexed with cyclin T or cyclin K, plays a role in promoting transcription and is highly expressed in solid tumors such as hepatocellular carcinoma, breast cancer, and hematological malignancies. However, reported CDK9 inhibitors have poor selectivity and are associated with various side effects including nausea, diarrhea, and abdominal pain. Therefore, 4-,5-,6-,7- azaindole was designed to develop an inhibitor with high selectivity and activity. Furthermore, to enhance the activity of the 7- azaindole, a lactamized 11-azapaulone was also designed. In this study, we will describe synthesis of azaindole and azapaullone core as new CDK9 inhibitors and their biological activity.

Poster Presentation : **MEDI.P-357**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

The Synthesis of Benzoindazole via Suzuki-Miyaura coupling and Aldol condensation cascade reaction.

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This study addresses the design and synthesis of novel kinase inhibitors centered around indazole. Indazole demonstrates diverse biological activities, particularly showing significant potential as kinase inhibitors. For example, FDA-approved drugs with the indazole core, such as Pazopanib, Axitinib, and Entrectinib, are used in the treatment of various conditions including kidney cancer, soft-tissue sarcoma, breast cancer, and non-small cell lung cancer.The goal of this research is to utilize the structural characteristics of indazole to synthesize compounds that can effectively inhibit various kinases. In this study, a convenient synthesis method for benzoindazole was achieved using Suzuki-Miyaura coupling and aldol condensation, which can be easily extended to a wide range of derivatives.

Poster Presentation : **MEDI.P-358**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Exploring Novel Ligands for the 5-HT$_7$ Receptor: A Computer-Aided Drug Discovery Approach for Autism Spectrum Disorder Treatment

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The 5-HT$_7$ (5-hydroxytryptamine, serotonin) receptor is a member of G-protein coupled receptor (GPCR) and is associated with various physiological processes in the central nervous system (CNS). Studies for the importance of serotonergic system in the early developmental stage and recent data lead 5-HT$_7$R to become a promising therapeutic target for autism spectrum disorder (ASD), a complex neurodevelopmental disorder with repetitive behavior and impaired social interaction. In this study, we carried out a computer-aided drug discovery (CADD) framework with a 5-HT$_7$ homology model to develop novel ligands. Using the ZINC and Chemdiv databases, we employed CDOCKER and LibDock calculation methods to predict the non-bond covalent interaction between a ligand and the receptor. The 54 compounds selected through the virtual screening were subsequently evaluated *in vitro*. Luminescent-based studies of the GPCR signaling pathway aided in defining the properties of the ligand, such as whether it acts as an agonist or antagonist. None of the compounds act as agonists over the signaling pathways such as the G$_s$, β-arrestin, and G$_{12}$ signaling. Remarkably, our rigorous screening protocols have led to the discovery of small molecules capable of blocking the G$_{12}$ downstream signaling cascades via 5-HT$_7$R without interfering others. We further evaluated the effects of compounds on Shank 3 Tg mice, resulting in an increase in repetitive behavior. Our findings clearly indicate that the development of an agonist for G$_{12}$ signaling is crucial, and 5-HT$_7$R appears to be a promising therapeutic target for ASD drug development.

Poster Presentation : **MEDI.P-359**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

The synergic effect of extracts mixture of *Ecklonia cava* and *Cinnamomum verum*

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The vegan beauty market is expected to grow by an average of 6.3% every year since 2021, to 27 trillion won in 2025. As a result, the beauty industry is avoiding animal ingredients from skincare to color cosmetics.A well known brown alga *Ecklonia* cava contains 6,6'-bieckol, dieckol, PFF, and fucoidan, and has cosmetic functions such as anti-inflammatory, antioxidative, and whitening activities. *Cinnamomum verum* is also known to contain cinnamic acid, cinnamic aldehyde, eugenol, and it has cosmetic functions such as anti-inflammatory, antioxidant, antibacterial, skin calming, and collagen production promotion activities. We conducted an initial study to develop functional materials by combining a marine algal extract and terrestrial plant extract to have diverse and enhanced biological activities. In the measurement of antioxidant activity, 70% ethanol extract of cinnamon showed slightly higher activity than that of *Ecklonia cava*. A mixture of the two extracts at 7:3 ratio showed highest radical scavenging activity. In the measurement of collagenase inhibitory activity, cinnamon extract showed better activity than *Ecklonia cava* extract, but a synergistic effect of increasing activity was observed in the complex extract mixture cinnamon and *Ecklonia cava* at 7:3 ratio.As a result, a combination of a marine algae extract and terrestrial plant extract at different ratios may enhance biological activities and potential to develop functional materials.

Poster Presentation : **MEDI.P-360**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

TWN-VS Method: A Novel Virtual Screening Method for Drug Discovery

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Virtual screening (VS) is extensively utilized in drug discovery to reduce both time and expenses. However, identifying the hotspots of proteins can be extremely challenging, especially for proteins where ligand bound crystal structures are not available. Our research group has been focusing on topological water network (TWN) analysis that enables the identification of water networks in the protein binding sites. TWNs are commonly observed in the hydrophobic pockets of proteins. Our previous studies suggest that highly dense TWN sites may indicate hotspots in the protein binding pockets. Earlier, our research group reported a TWN-based fragment screening (TWN-FS) method that suggests fragments through grouped TWN analysis within the protein binding site. However, similar to any other fragment-based drug design (FBDD) approaches, it is challenging to link fragments screened by TWN-FS. To address this problem, we propose TWN-VS, a novel screening method that can identify compounds rather than only fragments overlapping with the highly dense TWNs. We used this method to screen known kinase inhibitors. Our findings suggest that TWN-VS method has the potential to effectively screen compounds. Although some false positives can also be present in the screened compounds as this method does not consider pharmacophoric features. In the future, we plan to incorporate pharmacophoric features in the TWN-VS.

Poster Presentation : **MEDI.P-361**
Medicinal Chemistry
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Binding site similarity analysis for staurosporin-bound kinases using TWN-RENCOD method

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Staurosporin is a pan-kinase inhibitor that binds to multiple protein kinases. It effectively inhibits several kinases, exhibiting similar binding modes across various kinases as evidenced by crystal structures. However, conventional binding site similarity methods are not sufficient to explain its activity against diverse kinases. Consequently, it is important to consider the influence of binding site water molecules on the protein-ligand interactions which can introduce variability despite the similar ligand binding mode. We have developed a novel tool for comparing binding site similarity known as Topological Water Network Residue-based Encoding (TWN-RENCOD) method. This method calculates a distance matrix between atoms in the binding site residues and TWN centroids. Our study utilized co-crystal structures of staurosporin bound to 38 different protein kinases to evaluate the effectiveness of TWN-RENCOD in comparison to established binding site similarity calculation methods. By incorporating water into our analysis, TWN-RENCOD offers valuable insights into pan-kinase inhibitor analysis and may enhance our understanding of binding site similarities among diverse kinases.

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Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of a novel pharmacophore-based virtual screening approach using TWN analysis

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Pharmacophore-based virtual screening offers an effective method for identifying potential new compounds in the field of drug discovery. However, it typically relies on the three-dimensional structures of ligands or proteins, employing overlaying techniques for pharmacophore mapping. We are developing a novel pharmacophore approach that uses water molecules found within the binding site of a target protein. This approach involves performing molecular dynamics simulation on the unbound state of the protein and identifying topological water networks (TWNs) within its binding pocket. These TWNs are then treated as pseudo-ligands for constructing the pharmacophore model. Pharmacophoric features are assigned to these pseudo-ligands based on the chemical properties of nearby residues and the spatial distances between them. Genetic algorithm (GA) is then applied to these pseudo-ligands to define the pharmacophores. Furthermore, a non-superpositional technique referred to as the ultra-fast shape recognition with atom types (UFSRAT) method is utilized for comparative analysis between the generated pharmacophore model and query compounds.

Poster Presentation : **MEDI.P-363**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of Pan-kinase Inhibitors Using Topological Water Network Analysis

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Pan-kinase inhibitors exhibit a broad spectrum of inhibitory effects on various kinases, holding significant potential for effective therapeutic outcomes in diseases with multiple targets. We are involved in the development of new drugs using Topological Water Networks (TWNs). In our previous studies, we improved activity and selectivity of compounds against the target proteins by modifying substituents which overlap with TWNs observed in their binding sites. However, these studies were focused on selective kinase inhibitors. In this study, we aim to develop pan-kinase inhibitors by focusing on conserved TWNs and excluding the target-specific TWNs. We obtained crystal structures of 28 diverse protein kinases from the Protein Data Bank (PDB) and performed molecular dynamics simulation on them. Next, we analyzed TWNs and identified the most dense TWNs in their binding pockets. Subsequently, we docked fragments from a library into the binding sites of these kinases to discover fragments overlapping with dense TWNs. We plan to optimize these fragments to develop pan-kinase inhibitors.

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Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Ginsenoside Rh3 increases regorafenib-induced apoptotic cell death in hepatocellular carcinoma

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Ginsenosides are renowned for their diverse pharmacological effects, including their potential to combat various diseases, such as cancer. Meanwhile, regorafenib serves as a second-line treatment for advanced hepatocellular carcinoma (HCC), yet the emergence of drug resistance can diminish its anticancer efficacy. This study endeavors to establish a panel of ginsenosides, evaluating their activity in conjunction with regorafenib within HCC cell lines. Additionally, the underlying mechanism of the chosen ginsenoside's effects is explored. Through a screening process, synergistic effects were assessed, and an optimal combination of drug concentrations was determined using a synergy scoring tool. Additionally, ginsenoside Rh3 effectively enhances the susceptibility of HCC cells to the anticancer effects treated with regorafenib, achieved by promoting apoptosis. These findings were further validated through anti-cancer efficacy evaluations within an in vivo xenograft model. Collectively, this study demonstrates that the combination therapy of regorafenib and Rh3 exhibits enhanced therapeutic efficacy against HCC.

Poster Presentation : **MEDI.P-365**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Cannabidiol Enhances Cabozantinib-Induced Apoptotic Cell Death via Phosphorylation of p53 Regulated by ER Stress in Hepatocellular Carcinoma

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Cannabidiol (CBD), a primary constituent in hemp and cannabis, exerts broad pharmacological effects against various diseases, including cancer. Additionally, cabozantinib, a potent multi-kinase inhibitor, has been approved for treating patients with advanced hepatocellular carcinoma (HCC). Recently, there has been an increase in research on combination therapy using cabozantinib to improve efficacy and safety when treating patients. Here, we investigated the effect of a combination treatment of cabozantinib and CBD on HCC cells. CBD treatment enhanced the sensitivity of HCC cells to cabozantinib-mediated anti-cancer activity by increasing cytotoxicity and apoptosis. Phospho-kinase array analysis demonstrated that the apoptotic effect of the combination treatment was mainly related to p53 phosphorylation regulated by endoplasmic reticulum (ER) stress when compared to other kinases. The inhibition of p53 expression and ER stress suppressed the apoptotic effect of the combination treatment, revealing no changes in the expression of Bax, Bcl-2, cleaved caspase-3, cleaved caspase-8, or cleaved caspase-9. Notably, the effect of the combination treatment was not associated with cannabinoid receptor 1 (CNR1) and the CNR2 signaling pathways. Our findings suggest that the combination therapy of cabozantinib and CBD provides therapeutic efficacy against HCC.

Poster Presentation : **MEDI.P-366**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Cannabiorcol improves osteoarthritis by attenuating the expression of MMPs induced interleukin-1β via cannabinoid receptor 1

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Osteoarthritis (OA) is a degenerative joint disorder characterized by the progressive deterioration of joint cartilage, often accompanied by increased expression of matrix metalloproteinases (MMPs), which contribute to cartilage breakdown. Cannabiorcol, a derivative of Cannabis sativa, has shown potential anti-inflammatory effects. In this study, we employed in-silico analysis to investigate MMPs, including MMP-1, MMP-3, and MMP-13, revealing NF-kB and p38 as key regulators of MMPs mRNA expression. We hypothesized that cannabiorcol could mitigate MMPs expression by inhibiting the activation of NF-kB and p38 signaling pathways. Notably, cannabiorcol's effects were mediated through the cannabinoid receptor 1 (CNR1) signaling pathway. To evaluate cannabiorcol's efficacy, we treated rats with OA induced by mono-iodoacetate, observing reduced MMPs expression and improved OA following cannabiorcol treatment. These findings suggest that cannabiorcol may hold therapeutic potential against OA by mitigating MMPs expression through modulation of inflammatory pathways, highlighting its possible role as an OA treatment strategy.

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Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Design and Synthetic Derivatization of a Microtubule Inhibitor for Use as a Payload in Antibody-Drug Conjugates

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Microtubule inhibitors constitute the primary class of payloads used in antibody-drug conjugates (ADCs), which have regained attention in the field of medicinal chemistry. One such microtubule inhibitor recently approved by the FDA is tirbanibulin, which has been utilized as a first-in-class treatment for pre-cancerous actinic keratosis. It possesses a distinctive dual inhibitory mechanism, targeting both microtubules and Src. Our medicinal chemistry program aims primarily to enhance tirbanibulin’s potency for development as a payload in ADCs. We have focused on systemic variations of tirbanibulin's structure, which can be categorized into three motifs: A- and C-rings and the morpholine part. Based on the cocrystal structure of tirbanibulin in tubulins, we strategically synthesized derivatives of tirbanibulin and evaluated their in vitro mechanisms of action (MOAs). Our representative analogs exhibited promising cytotoxicity profiles (single-digit nanomolar IC50), accompanied by notable induction of cell cycle arrest at the G2/M phase and inhibition of p-Src levels. Moreover, these derivatives feature a linker appendage site enabling attachment to antibodies, thus allowing for their utilization as payloads in ADCs. The results and investigative story will be detailed in the poster.

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Poster Presentation : **MEDI.P-368**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Synthesis and biological evaluation of flavonoid based TSLP inhibitors.

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Thymic stromal lymphopoietin (TSLP) is a proinflammatory cytokine is involved in various allergy disorders mediated by differentiation and proliferation of type2 helper cell (Th2) responses such as asthma and other atopic diseases. TSLP forms tight ternary complex binding with the TSLP receptor (TSLPR) and interleukin receptor-α (IL-7Rα) leading to the activation of complex intracellular cascade, which ultimately release of pro-inflammatory mediators. Here, we designed and synthesized biphenyl flavonoid derived small molecule inhibitor of the TSLP signaling pathway. Flavonoid derivatives were constructed by applying the Algar-Flynn-Oyamada reaction. Synthesized compounds obtained in moderate to good yields (44-61 %). In vitro studies showed that KB-4606 and KB4604 blocked the interaction between TSLP and TSLPR in a dose dependent manner with higher potency. Kinetic solubility results reveal that KB-4606 showed better aqueous solubility. Further, KB-4606 better metabolic stability in both human and mouse studies. Currently, Structure-activity relationship and in vivo assay are in progress.

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Efficient estimation of protein solvation free energy and vibration entropy using graph neural networks

Yeseul Oh

Seoul National University, Korea

Protein free energy prediction is an important area of research in drug discovery and bioinformatics. The widely used computational method for calculating free energy, MMPBSA, is reliable but computationally expensive. To address this issue, AI-based approaches have emerged as a promising alternative for predicting protein structure and function. In this study, we propose a novel framework for predicting free energy of the given protein structures by training a Energy-based Graph Neural Network model. We hypothesize that 3D structures of proteins must contain physical/biological information which can be extracted by AI models. To develop the model, we obtained protein structures-energy pairs through molecular dynamics simulations and MMPBSA methods, respectively. Our method has the potential to significantly reduce the time required to calculate free energy, making it a valuable tool in drug development and other areas of research. A successful AI-based model for predicting protein free energy has far-reaching implications for drug discovery and other areas of research. It could provide rapid compound structure information and predict in-silico protein binding ability, suggesting new drug candidates, and predict drug interactions to reduce trial and error in the clinical trial design stage. Thus, our study could contribute significantly to the development of new drugs and therapies.

Poster Presentation : **MEDI.P-370**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

In-silico Studies of Ligand Binding Sites on 3R-, 4R-, and mixed 3R/4R Tau Fibril Folds.

Lizaveta Gotina, Ae Nim Pae[1,*]

Department of Bio-Medical Science and Technology, University of Science & Technology, KIST School, Korea
[1]*Brain Science Institute, Korea Institute of Science and Technology, Korea*

The aggregation of the microtubule-associated protein tau into pathological oligomers and neurofibrillary tangles underlies the pathogenesis of numerous neurodegenerative disorders collectively termed tauopathies. These diseases include Alzheimer's disease (AD), progressive supranuclear palsy (PSP), chronic traumatic encephalopathy (CTE) , corticobasal degeneration (CBD), Pick's disease (PiD) and others. Recently, advances in cryo-EM revealed that distinct structures of tau filaments are formed depending on the predominantly aggregating tau isoform, opening the opportunity to the design of disease-specific tau-binding ligands.However, the precise binding modes of small molecules to tau fibrils remain largely elusive. In this study, we employed 200 ns all-atom molecular dynamics (MD) simulations to probe the conformational dynamics and identify potential cryptic binding sites within tau fibrils associated with distinct tauopathies. Specifically, we investigated the structures of 3R-, 4R-, and mixed 3R/4R tau fibrils, represented by the PiD, PSP, and AD folds, respectively. Simulations were performed with separate tau fibrils and in the presence of tau-binding molecules. Our findings reveal distinct ligand binding sites in each tau structure, shedding light on the molecular interactions between small molecules and tau fibrils. Importantly, these results expand the current understanding of small molecule binding to tau fibrils beyond the limited scope of available cryo-EM structures of tau bound to positron emission tomography (PET) tracers. Moreover, our study offers new avenues for drug discovery in the field of neurodegenerative diseases, providing insights for the rational design of tau-binding ligands tailored to specific tauopathies.

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Poster Presentation : **MEDI.P-371**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of fluorescent imaging probes for selective detection of tau protein and Aβ in Alzheimer's disease

Sunhwa Jung, Su-Jin Gu[1], Sun-Joon Min[2,*]

Department of Applied chemistry, Hanyang University, Korea

[1]*Department of Applied Chemistry, Hanyang University, Korea*

[2]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Alzheimer's disease (AD) is a neurodegenerative disease characterized by cognitive decline and memory impairment. With the rapid increase of the population of AD patients, the disease has become a significant economic and social burden throughout the world. Currently, clinically approved treatments for Alzheimer's disease only delay the progression of the disease or alleviate symptoms. Therefore, the early diagnosis of AD patients is important to prevent the disease from becoming severe. Amyloid-beta (Aβ) peptide deposition and hyperphosphorylated tau protein are considered critical pathological hallmarks in AD. Chemical probes to visualize these biomarkers have been developed to test the progression of the disease, but it is still needed to discover novel imaging probes for the identification of a precise disease stage.In this work, we present the design and synthesis of NIR fluorescent probes that selectively detect Aβ plaques and tau aggregates based on differences in the linker connecting the electron donor and acceptor. New donor-π-acceptor compounds OMCL20-1, 20-2, and 20-3 with different types of π-bond linkers were synthesized, and in vitro evaluation of their ability to bind Aβ or tau aggregates selectively were performed. The results showed that OMCL20-1 series showed fluorescence enhancement in the presence of Aβ aggregates, while OMCL20-2 and OMCL20-3 displayed high fluorescence signal in the presence of tau aggregates, with maximum emission values in the NIR range. In particular, OMCL20-3 series, which contains improved donor and acceptor, has been shown to bind more selectively to tau aggregates than to Aβ aggregates compared to ThS, a known AD fluorescent probe.

Poster Presentation : **MEDI.P-372**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

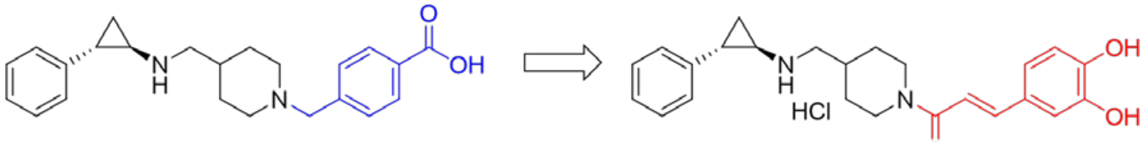
Synthesis and Biological Evaluation of Tranylcypromine analogs as a Potent Inhibitor of LSD1 Related Osteoclast Differentiation Activity

Eun Rang Choi, Se Myeong Choi, A Young Jung[1], Jong Hyun Cho[*]

Dong-A University, Korea

[1]*Health science, Dong-A University, Korea*

Bone homeostasis is maintained by osteoclastic bone resorption and osteoblastic bone formation. It was reported that LSD1 deficiency led to inhibition of osteoclast differentiation. Therefore, new tranylcyptomine-methylpiperidine-caffeic acid (TCP-MP-CA) analogs was designed from a scaffold of GSK2879552, which is one of the moderate LSD1 inhibitors. Fifteen TCP-MP-CA analogs were synthesized by using reductive amination and coupling reaction as the key reactions. Among prepared analogs, TCP-MP-CA analog (4) showed the most potent activity (IC_{50} 0.14 μM, CC_{50} > 100 μM) against osteoclastogenesis *in vitro*. In the co-crystal structure, it was confirmed that compound 4 binds to the LSD1/CoREST complex through FAD to reduce LSD1 demethylation enzyme activity. Ultimately, TCP-MP-CA (4) was discovered as a novel inhibitor of osteoclastogenesis.



GSK-2879552
IC_{50} = 0.37 μM

4
IC_{50} = 0.14 μM

Poster Presentation : **MEDI.P-373**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

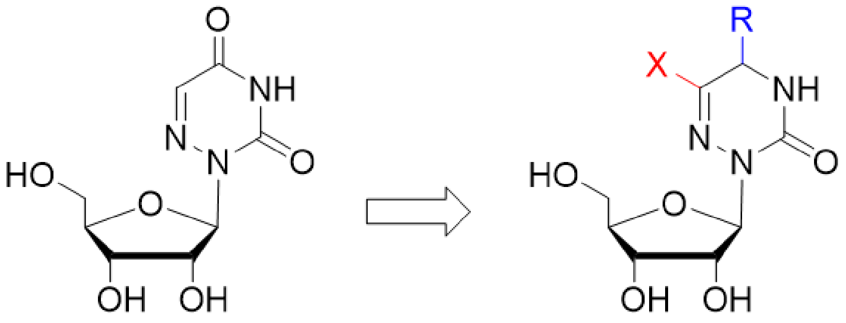
Synthesis and Evaluation of 6-Azauridine Analogs against DENV-2 and West Nile Virus Replicon

A Young Jung, Eun Rang Choi, Se Myeong Choi, Jong Hyun Cho*

Health science, Dong-A University, Korea

6-Azauridine(6-AZA), a inhibitor of orotidine monophosphate decarboxylase, showed antiviral activity against several viruses including dengue virus (DENV), West Nile virus (WNV), coronavirus (SARS-CoV-2). Despite of a broad-spectrum antiviral activity, 6-AZA has limitation of low bioavailability and high toxicity *in vivo* to develop an antiviral agent. Therefore, we designed various 6-AZA analogs to improve its toxicity and activity. First, we prepared 6-azauracil analogs with halogen atom instead of hydrogen at the C-5 position of 6-azauracil by using halo succinimides, respectively. The Vorbrüggen reaction of two 5-halo-6-azauracils with D-ribose derivative to afforded their corresponding 5-halo-6-AZA analogs in 87-90% yield. Finally, the carbonyl group at the C-4 position of 5-halo-6-AZA analogs were substituted with NH_2, NHOH to give new 6-AZA analogs after removal of the protecting groups. Eleven 6-AZA analogs are screening for DENV-2, and WNV replicon BHK cells.

Figure1.



6-Azauridine

5-Halo-6-azauridine analogs

R = OH, NH_2, NHOH
X = I, Br, H

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Poster Presentation : **MEDI.P-374**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

DNA-Compatible Copper-Mediated Synthesis of *N*-Sulfonyl Amidines for DNA-Encoded Libraries

YeonHee Lee, Seok Woo Lee*, Hyunjin Kim[1,*], Minseo Choi[1]

College of Pharmacy, Chungnam National University, Korea
[1]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

The DEL (DNA-encoded library) technology utilizes DNA-based unique barcodes to rapidly screen large-scale libraries. This technique was proposed by Brenner and Lerner in 1992 and is increasingly important due to its efficiency and cost-effectiveness in identifying active compounds compared to conventional screening methods like HTS (High-Throughput Screening). However, DEL is typically limited in library construction because organic molecules are generally synthesized while bound to single or double-stranded DNA. Therefore, expanding the structural diversity of DEL through novel DNA-compatible reactions remains a significant challenge. *N*-sulfonyl amidines, characterized by various physiological activities, serve as functional groups, with amidine derivatives being useful intermediates in the synthesis of diverse heterocyclic compounds and metal complexes. In this study, we propose a copper-mediated *N*-sulfonyl amidine synthesis applicable to the construction of DEL and suitable for a wide range of substrates.

Poster Presentation : **MEDI.P-375**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Discovery of novel YAP-TEAD interaction inhibitors for colorectal cancer treatment

On-Yu Kang, Jiyoung Hyun, Seong Jun Park, Hwan Jung Lim[*]

Data Convergence Drug Research Center, Korea Research Institute of Chemical Technology, Korea

The Hippo pathway is known to have tumor-suppressive role, and dysregulation of the Hippo signaling pathway result in tumorigenesis and overgrowth of tumor. Although most promising druggable target of the Hippo pathway is to inhibit binding YAP, a transcriptional co-activator, and TEADs, transcriptional factor in nucleus, drug candidates selectively targeting YAP-TEAD are still lacking. In this study, we identified drug-like hit compound screened from integrated 3D database, based on structural interface between YAP-TEADs. We synthesized lead compounds that showed solid structure-activity-relationship (SAR) and promising anti-cancer activities in animal models with almost no side-effects. Selective binding of an inhibitor with TEAD proteins was confirmed through various biochemical assays. We suggest that our compounds had a potential to be investigated as a drug candidate targeting YAP-TEAD binding for cancer treatment.

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Poster Presentation : **MEDI.P-376**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Design and synthesis of selective JAK1 Inhibitors for the treatment of autoimmune diseases

Santosh shivanand Raikar, Pilho Kim[1,*]

Medicinal chemistry and Pharmacology, University of Science & Technology, India

[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Janus kinase 1 (JAK1) inhibitors have emerged as a promising class of drug target for the treatment of autoimmune diseases. Autoimmune and inflammatory conditions are widespread and come in many forms, capable of impacting any part of the body. Thus, JAK inhibitors are essential for the treatment of autoimmune diseases, offering significant benefits to patients with conditions, such as rheumatoid arthritis, ulcerative colitis, and psoriasis. However, concerns over the safety and selectivity of these drugs have been raised. Several JAK1 inhibitors have been developed and are currently in clinical trials for the treatment of autoimmune diseases. Tofacitinib and baricitinib have been approved by the US FDA for the treatment of rheumatoid arthritis and atopic dermatitis, respectively. While non-selective JAK inhibitors could lead to off-target effects and potential toxicities, selective inhibitors could offer greater specificity and reduce side effects. Filgotinib, a promising selective JAK1 inhibitor, has shown encouraging results in early clinical trials and may offer more safe and effective alternative to the regimens including JAK inhibitors. To discover JAK1-selective inhibitors, novel compounds have been designed derived from filgotinib. Optimization processes, biological activities, ADME/Tox profiles will be presented. Finally, in vivo efficacy studies of selected compounds using a collagen-induced arthritis (CIA) model will be discussed.

Poster Presentation : **MEDI.P-377**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Macrocyclic compounds as GLS Inhibitor for anticancer agents 2

YeongJu Kwon, Kwangho Lee[*], Rajath Cyriac[1]

New Drug Information Technology Research Center, Korea Research Institute of Chemical Technology, Korea

[1]*New Drug Information Technology Research Center, University of Science & Technology, Korea*

Glutamine-addicted cancer metabolism is recently recognized as novel cancer target especially for KRAS and KEAP1 co-occurring mutations. Selective glutaminase1 (GLS) inhibition was reported using BPTES which has novel mode of allosteric inhibition. However, BPTES is a highly hydrophobic and symmetric molecule with very poor solubility which results in suboptimal pharmacokinetic parameters and hinders its further development. To identify more drug-like GLS inhibitors via systematic structure−activity relationship (SAR) analysis of BPTES analogs, we have disclosed our novel reverse-amide macrocycles for GLS inhibition with conclusive SAR analysis on the core, core linker, and wing linker, respectively. As a part of follow-up study, we present amide macrocycles for GLS inhibition with unique SAR analysis. Selected molecules resulted in reduction in intracellular glutamate levels in LR (LDK378-resistant) cells which is consistent to A549 and H460 cells viability result.

Poster Presentation : **MEDI.P-378**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Structure-based drug design approach and synthesis for a new class of nucleoside A_{2A} adenosine receptor antagonist as promising immune-oncology agents

Gibae Kim

College of Pharmacy, Seoul National University, Korea

In this study, we focused on the A_{2A} adenosine receptor (A_{2A}AR), a key subtype within the adenosine receptors, as a crucial target in the development of immune-oncology therapies. Previous approaches to develop A_{2A}AR antagonists have predominantly involved the use of modified purines or related heterocyclic structures, reflecting their natural affinity to the adenosine-based endogenous ligand. A common strategy has been to eliminate the ribose group to transition the compound's function from an agonist to an antagonist, highlighting the pivotal role of the ribose-induced interaction in activating the receptor. Our research successfully developed a nucleoside-based antagonist for A_{2A}AR through structure-based drug design approach. We synthesized a series of 22 different molecules following an extensive structure-activity relationship (SAR) analysis, employing Vorbrüggen glycosylation and selective palladium-catalyzed cross-coupling reactions as key steps. The lead compound emerged with a high affinity for A_{2A}AR, exhibiting a K_i value of 7.7 nM and It completely inhibited cAMP production via A_{2A}AR signaling. Additionally, this compound was evaluated for its anti-cancer effect in vivo, where it showed a synergistic effect in combination with a mAb immune checkpoint inhibitor. Our findings introduce a new class of nucleoside-based A_{2A}AR antagonists, identified through SAR and structural analysis, with potent in vivo anti-proliferative effect, offering valuable insights into receptor activation mechanisms and potential therapeutic applications in immune-oncology.

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Poster Presentation : **MEDI.P-379**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of a novel nano-reactor assembly with 8-(N-phenylhexanamido) naphthalene-1-sulfonate, HBF4 and Fe(BF4)2, and its application to the amination of alcohol

Waqar Ahmed

Bionano Chemistry Lab (BNCL), Department of Bionano Engineering, Korea

Diverse artificial vesicles have been employed for many biomedical applications, such as drug carriers, bioreactors and gene delivery. These vesicular assemblies have not been fully studied for development of organic reactions in water, although their micellar counterparts have enormously been used for the same purpose as a green alternative system. We introduce a vesicle-like nano-reactor assemblies formed by a novel amphiphilic catalyst (8-(N-phenylhexanamido)naphthalene-1-sulfonate (Cat-3)), HBF4 and Fe(BF4)2 in water and their use as nano-reactors for development of dehydrative amination of alcohols in aqueous solution. These assemblies showed a significantly enhanced performance than the micellar catalysts, such as sodium dodecyl sulfate (SDS), sodium dodecylbenzene sulfonate (SDBS), and Brij-35 for the dehydrative amination of various alcohols. The dehydrative amination reaction utilizing Cat-3-HBF4-Fe(BF4)2-based assemblies in water was favorable owing to its efficient and environmentally-friendly set-up, easily available starting materials and non-toxic catalysts. The present method was also applied as a key step for the gram-scale total synthesis of the FDA-approved drug, naftifine. The assemblies were characterized through dynamic light scattering (DLS), ζ-potential, transmission electron microscopy (TEM) and confocal microscopy (CLM).

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Poster Presentation : **MEDI.P-380**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

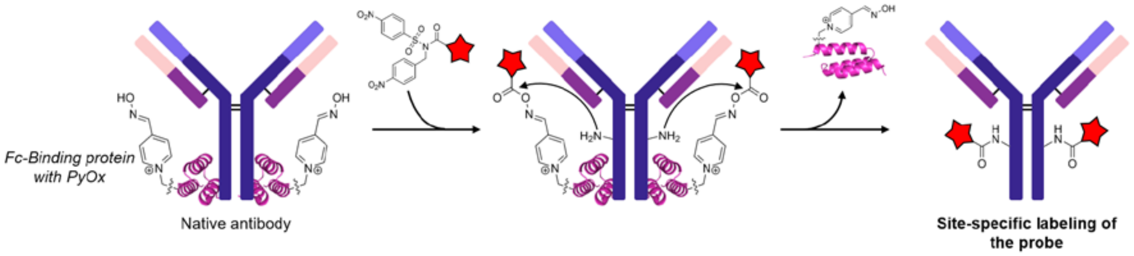
Affinity-Directed Site-Specific Protein Labeling and Its Application to Antibody-Drug Conjugates

Sooin Kim, Hyun Soo Lee[1,*]

Chemistry, Sogang University, Korea

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

Chemically modified proteins have diverse applications; however, conventional chemo-selective methods often yield heterogeneously labeled products. To address this limitation, site-specific protein labeling holds significant potential, driving extensive research in this area. Nevertheless, site-specific modification of native proteins remains challenging owing to the complexity of their functional groups. Therefore, a method for site-selective labeling of intact proteins is aimed to design. In this study, a novel approach to traceless affinity-directed intact protein labeling is established, which leverages small binding proteins and genetic code expansion technology. By applying this method, a site-specific antibody labeling with a drug, which leads to the production of highly effective antibody-drug conjugates specifically targeting breast cancer cell lines is achieved. This approach enables traceless conjugation of intact target proteins, which is a critical advantage in pharmaceutical applications. Furthermore, small helical binding proteins can be easily engineered for various target proteins, thereby expanding their potential applications in diverse fields. This innovative approach represents a significant advancement in site-specific modification of native proteins, including antibodies. It also bears immense potential for facilitating the development of therapeutic agents for various diseases.


Fc-Binding protein with PyOx
Native antibody
Site-specific labeling of the probe

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Poster Presentation : **MEDI.P-381**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Catalyzing Breakthroughs: The Next Wave of Rapid and Efficient Drug Discovery

Jiwoong Lim, Kenneth H. Pearce*

Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, United States

Traditional drug discovery, heavily reliant on small molecule therapeutics and structure-activity relationship (SAR) studies, often faces the challenge of time-consuming synthesis and individual compound testing. While high-throughput screening techniques and virtual screening based on pharmacophore studies have expedited the hit compound identification process, they still have limitations, particularly in addressing 'undruggable' targets. Leveraging advanced display technologies for peptide drug development offers a promising solution. By integrating biomolecular display systems with next-generation sequencing, we can rapidly and efficiently identify peptide drug candidates with high affinity, selectivity, and low toxicity for previously undruggable targets. This presentation will explore various display technologies, including mRNA and Phage display, and discuss their practical application in the early stages of drug discovery, mainly focusing on oncological targets. Furthermore, focused DNA-encoded library studies will be introduced to develop drug-like peptidomimetics, capturing the best features of small molecules and peptides.

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Poster Presentation : **MEDI.P-382**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Bioreductive fluorescent probes as a platform for development of cleavable linkers targeting hypoxia tumors and prodrugs synthesis.

Nhat Quynh Le, **Dong-Jo Chang**[*]

Department of Pharmacy, Suncheon National University, Korea

Antibody–drug conjugates (ADCs) are currently receiving substantial attention as an alternative class of therapeutics allowing targeted therapy and reducing the impact on healthy cells for the clinical treatment of cancer. The linker is one of the critical factors determining the efficacy and toxicity of ADCs. The choice of linker in ADC design can significantly affect the efficiency, specificity and safety profile of the ADC. However, the ability to release payload and plasma stability of cleavable linkers are generally evaluated by complex in vivo techniques by LC-MS, and the design of a clinically applicable linker is still a challenging and time-consuming task. Hypoxia is a common feature of many solid tumors with underlying cellular pathways that promote tumor survival. As a result, hypoxia is strongly associated with poor prognosis and resistance to chemotherapy and radiotherapy. In this work, novel “turn on” fluorescent probes diversely linked to o, m or p-nitrobenzyl and di-nitrobenzyl spacers have been developed in order to screen different cleavable linker for ADCs targeting hypoxia. The regio- and stereo-electronic effect of nitro group in benzyl spacer on the release of fluorophore has been studied by the analysis of kinetics during nitroreductase (NTR) reaction. Also, temperature and pH stability, and selectivity tests for various biomolecules were conducted to develop a cleavable linker with enough stability and selectivity. Fluorescent probes with p-nitro and o, p-dinitrobenzyl spacers showed the highest performance in enzyme assays and were chosen to develop prodrugs which can release a camptothecin derivative with nanomolar cytotoxicity by the reaction with NTR under hypoxic condition.

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Poster Presentation : **MEDI.P-383**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of new target protein small molecules as a novel class of H_2O_2 scavenger for treatment of Alzheimer's Disease

Elijah Lee, Ki Duk Park[1,*]

Center for Brain Disorders, Korea Institute of Science and Technology, United States
[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Alzheimer's disease (AD) is the most common form of dementia and is a progressive neurodegenerative disease characterized by memory loss. In the AD brain, reactive oxygen species (ROS) levels are significantly higher than that of healthy aging brain. Hydrogen peroxide (H_2O_2) is a representative ROS that causes oxidative stress and is a product of many different metabolic pathways in AD1. We recently investigated the mechanism of action of the drug HTPEB, which is effective in scavenging H_2O_2 in neurodegenerative disease mouse model. In this study, we aim to optimize the efficacy and drug-like properties of HTPEB to develop a novel H_2O_2 target candidate for treatment of AD. We synthesized a series of novel compounds and evaluated the H_2O_2 scavenging activity using an optimized in vitro assay system. Among them, KDS12025 exhibited three times the efficacy of HTPEB (EC_{50}: 0.0449 µM to 0.1551 µM, respectively) and also showed favorable microsomal stability (57.6% in human during 30 min to

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Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Discovery of Heterocyclic Structure-Based Novel P2X3 Receptor Antagonists

Ga-Ram Kim, Yong-Chul Kim*

School of Life Sciences, Gwangju Institute of Science and Technology, Korea

P2X3 receptor, an ATP ligand-gated cation channel predominantly expressed in C- and Aδ- primary afferent nerves, has been reported as the drug target for various neurological diseases such as neuropathic pain and chronic cough. Aiming to develop novel and selective P2X3R antagonists, tetrazolopyrimidine-based hit compound was optimized through structure‒activity relationship studies with modifications at the tetrazole core skeleton as well as side chain substituents. The finally optimized compound, with cyclopropane substituted triazolopyrimidine core structure, showed potent P2X3R antagonistic activity with an IC50 value of 54.9 nM with 20-fold selectivity vs P2X2/3R, which is responsible for the taste-loss side effect and low antagonistic activities at other P2XR subtypes. An in-vivo study in the spinal nerve ligation neuropathic pain rat model showed an antiallodynic effect in a dose-dependent manner.

Poster Presentation : **MEDI.P-385**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Discovery of hit compound for psoriasis targeting peripheral tissue CB1 receptors

Wonjin Park, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Recently, the number of patients with psoriasis, an inflammatory skin condition, has been increasing. This condition poses difficulties for patients due to high treatment costs and frequent relapses. To address this unmet needs, we envisioned to find hit compounds via revisit the 1st generation FDA-approved CB1R antagonist, rimonabant, as a potential alternative to conventional interleukin therapy for psoriasis. To address the issue of blood-brain barrier (BBB) penetration associated with rimonabant, we are aiming to discover antagonists that exhibits similar antagonistic properties, but reduced BBB penetration, compared to rimonabant.

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Poster Presentation : **MEDI.P-386**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Discovery of indolizine derivatives that synergistically enhance the activation of the STING pathway by cGAMP

Eunsu Kim, Wonjin Park[1], Eunha Kim[*]

Department of Molecular Science and Technology, Ajou University, Korea

[1]*Ajou University, Korea*

Abstract: Immunotherapy have revolutionized tumor treatments, yet the clinical response rates, especially in cold tumors, remain suboptimal. The tumor microenvironment often hinders immune cell infiltration, making these tumors less responsive to immune system. Converting cold tumors into hot tumors by triggering an active immune response can enhance immunotherapy efficacy. The cGAS-STING pathway activation represents a crucial mechanism in the cancer immunity cycle, holding promise for immuno-oncology. Despite ongoing trials with STING agonists, current limitations include poor pharmacokinetics, physicochemical properties, and potential adverse effect. There is a growing need for improved modalities to activate the STING pathway for effective cancer therapy.In this study, we present indolizine derivatives demonstrating synergistic activation of the STING pathway in conjunction with cGAMP. Combined treatment of our compound with a low dose of cGAMP significantly increased ISRE activity. Increased STING stability was demonstrated with the compound-cGAMP combination. In vivo test, co-administration induced significant tumor regression. Our findings suggest that the indolizine core skeleton holds promise as a novel chemical entity for STING activation, addressing current limitations in STING agonist development.

Poster Presentation : **MEDI.P-387**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Discovery of NLRP3 inflammasome modulators for treatment of inflammatory diseases

Kyungmin Kim, Sun-Joon Min[1,*]

Department of Applied Chemistry, Hanyang University, Korea

[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

The NLRP3 (NOD-, LRR- and pyrin domain-containing protein3) inflammasome, a multimeric protein complex, plays a crucial role in instigating a form of cell death associated with inflammation and triggering the release of proinflammatory cytokines like IL-1β and IL-18. Irregular activation of NLRP3 has been associated with various inflammatory diseases, including Cryoprin syndrome, Alzheimer's disease, diabetes, and atherosclerosis. Over the recent decades, inflammasomes have gained significance as a crucial component of the innate immune system, orchestrating the host's immune homeostasis. In this study, we found that the peptide fragment 72FYAQFVQALS81 and 401TLTGRPLIGNGANG414 derived from Mycobacterium tuberculosis (MTB) secretion interact with the domain of CD86, CD163 NLRP3, regulating the release of both proinflammatory cytokines IL-1β and IL-18. Based on the structure of this peptide motif, we designed N-heterocyclic derivatives as peptide-mimetic small molecules through in silico pharmacophore generation. We performed docking studies of the designed molecules to the X-ray crystal structure of the NLRP3 protein, which binds to MCC950, a potent NLRP3 inhibitor (PDB: 8ETR). While inhibitor candidates were docked at NLRP3 NACHT domain, a binding site of MCC950, activator candidates were docked at the newly designated binding site of NLRP3 PYD domain. The synthesis and in-vitro evaluation of the compounds with high CDOCKER energy scores in the docking study showed that they not only modulate the NLRP3 inflammasome function, but also reduce reactive inflammatory cytokine production. Among them, the most potent inhibitor was selected and conjugated with M1 macrophages targeting peptide to afford peptide-drug conjugate, which was further evaluated in

vitro as an anti-inflammatory agent. In this presentation, we will provide a discovery process for peptide-derived small molecules targeting NLRP3 inflammasome for the treatment of inflammatory diseases.

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Poster Presentation : **MEDI.P-388**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Discovery of hit compounds targeting the peripheral tissue cannabinoid 1 receptor (CB1R) for psoriasis treatment

Minyoung Lee, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

The control of Cannabinoid 1 Receptor (CB1R) has been recognized as a fundamental approach for treating inflammatory diseases, but concerns about neuropsychiatric side effects have driven the need for peripheral tissue specific CB1R antagonists. In this study, a structure-activity relationship analysis on a known CB1R antagonist revealed a superior compound with enhanced affinity and inhibition exclusively for CB1R. Importantly, the predicted blood-brain barrier penetration rate was reduced compared to its predecessor, minimizing the risk of neuropsychiatric side effects.

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Poster Presentation : **MEDI.P-389**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Exploring Amidobenzimidazole Derivatives for Enhanced Cancer Immunotherapy via Stimulator of Interferon Genes Modulation

Sohyeon Jeong, Gyu-Yong Song*, Hyejin Kim[1,*]

College of Pharmacy, Chungnam National University, Korea
[1]*Infectious Diseases Therapeutic Research Center, Korea Research Institute of Chemical Technology, Korea*

Stimulator of interferon genes (STING) agonists hold significant promise as immunomodulatory agents for cancer therapy. Herein, we present the discovery of a novel orally available STING agonist, SAP-04, exhibiting potent immunomodulatory effects for cancer therapy. Through the optimization of the amidobenzimidazole core with diverse pyridine-based heterocyclic substituents, we identified a monomeric variant demonstrating superior STING agonistic activity compared to its dimeric counterpart. SAP-04 efficiently induced cytokine secretion associated with innate immunity via direct binding to the STING protein, initiating sequential signal transduction along the STING signaling pathway and eliciting type I interferon (IFN) responses. Subsequent pharmacological validation, both in vitro and in vivo, underscored the potential utility of SAP-04 as an immunomodulatory agent for cancer therapy in vivo. Notably, significant in vivo anticancer effects were observed in a 4T1 breast tumor syngeneic mouse model following oral administration of the compound. Our findings suggest a promising strategy for the development of synthetically accessible monomeric variants as orally available STING agonists, offering new avenues for cancer immunotherapy.

Poster Presentation : **MEDI.P-390**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Studies on the synthesis and chemical transformations of acrolein and its acetal forms

Ye Eun Kim, Eunkang Cho, Hyemin Son, Sang Hyup Lee[*]

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Acrolein (2-propenal, CH_2=CHCHO) is the simplest unsaturated aldehyde. Acrolein is a highly electrophilic compound due to the presence of carbonyl group and conjugated vinyl group. The reactivity makes acrolein readily react with several nucleophilic biomolecules, leading to deleterious effects on human and bacteria. Although acrolein is known to be harmful for human, acrolein was required for the industrial demand and biological purposes. The biological activities of acrolein acetal forms have not been extensively investigated yet, but their uses as building blocks for the total synthesis of compounds with medicinal properties were reported. In this study, we focused on the synthesis and derivatization of acrolein, specifically concentrating on its acetal forms. We also covered the synthesis of acrolein acetal forms using appropriate starting materials. We aimed to highlight the significance of these useful molecules for both industry and medicinal chemistry through comprehensive investigations on the chemical reactions of acrolein and its acetal forms.

Poster Presentation : **MEDI.P-391**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of a Methylene Blue Conjugated EuKf Derivative for the PSMA-Targeted Photodynamic Therapy

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Purpose: PSMA is a good biomarker for diagnostics and treatments of prostate cancer (PC) due to its expression level being correlated with the progression of the disease. Photodynamic therapy (PDT), which utilizes photosensitizers (PS) that generate reactive oxygen species (ROS) upon exposure to light. PDT holds the advantage of yielding a potent therapeutic efficacy while concurrently minimizing the occurrence of adverse effects. In this work, we have developed a novel PSMA-targeted methylene blue (MB)-conjugated EuKf derivative for PDT in PC.Methods: We used the EuKf derivative which was confirmed its binding affinity through a competitive binding assay with 125I-MIP-1095 as the PSMA-targeted moiety. Based on EuKf, we synthesized the MB-conjugated EuKf derivative (PSMA-MB) and then isolate it using HPLC. PSMA-MB was confirmed through NMR and LC-MS assay. PSMA expression levels of LNCaP (PSMA+) and PC-3 (PSMA-) cells were measured by western blot. Confocal imaging and PDT study with PSMA-MB was performed to assess its PSMA targeting and PS efficacy.Results: The EuKf derivative has the highest MM-GBSA score (-68.18 kcal/mol) and binding affinity (IC50 = 2.3 nM), surpassing other compounds. Confocal microscopy revealed that PSMA-MB has higher uptake in LNCaP cells compared to PC-3 cells and showed PSMA-specific uptake in the presence of the blocking agent. In addition, a relative increase in ROS generation was observed in LNCaP cells following 660 nm laser irradiation.Conclusion: We developed the novel PSMA-targeted theranostic agent that showed effective PSMA-specific fluorescent imaging as well as potential PDT functionality in PC. Further evaluations of PSMA-MB are ongoing to identify more positive potential for PDT in PC.

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Poster Presentation : **MEDI.P-392**
Medicinal Chemistry
Exhibition Hall 2 FRI 11:00~13:00

Integrating Click Chemistry into PROTACs: Facilitating Antibody Conjugation for Enhanced Therapeutic Targeting

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Selective degradation of target proteins using proteolysis targeting chimeras (PROTACs) is being considered as a promising alternative to conventional protein inhibition. PROTACs selectively degrade specific proteins, minimizing side effects and enhancing therapeutic stability. PROTACs offer a versatile approach for the targeted modulation of diverse protein targets, thereby presenting avenue for the development of therapeutics. Current PROTACs are comprised of a target protein binder, an E3 ligase responsible for mediating ubiquitination of the target protein, and an interconnecting linker facilitating the conjugation between these two molecular entities. However, PROTACs encounter difficulties in synthesis due to the molecular complexity and issues related to low solubility. To overcome these challenges, we employ a strategy involving the assembly of small molecules into bifunctional complex, utilizing biorthogonal click reaction. Additionally, by harnessing the interaction between trans-cyclooctene (TCO) with tetrazine, we conjugated a tetrazine tag to the E3 ligase and a TCO tag to the target protein binder for the intracellular assembly of smaller molecular entities. Furthermore, these click-based PROTACs are amenable to conjugation with antibodies through cleavable linkers. In conclusion, the resultant degrader-antibody conjugates (DACs) demonstrate the capacity to selectively degraded target proteins by engaging cell surface antigens, thereby achieving enhanced selectivity.

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Poster Presentation : **MEDI.P-393**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of UMP Kinase (pyrH) Inhibitor as a Novel Class of Broad-Spectrum Antibiotics

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Antimicrobial resistance is a significant global public health challenge due to the overuse of antibiotics. Methicillin-resistant Staphylococcus aureus (MRSA) is a prominent multi-drug-resistant bacterium that causes difficult-to-treat infections in humans. Novel antibiotics are urgently needed to combat antibiotic resistance effectively. We screened our proprietary in-house compound library for antibacterial activity against MRSA. DN201511 was identified as a promising candidate with a MIC50 of ~5 μM against various MRSA strains. Notably, DN201511 exhibited bactericidal activity faster than Vancomycin does by disrupting abnormal molecules within MRSA. Transcriptomic analysis of DN201511-treated MRSA led to the discovery of a novel target, UMP kinase (pyrH), in the pyrimidine biosynthesis pathway. DN201511 inhibited pyrH with an IC50 of ~5 μM, a recombinant protein of Staphylococcus aureus. Additionally, DN201511 displayed a submicromolar activity against Vancomycin-resistant Enterococci (VRE) and demonstrated a remarkable synergistic effect when combined with colistin against Pseudomonas aeruginosa (PAO1, a Gram-negative bacteria). We synthesized over 170 compounds in our efforts for lead optimization, aiming to develop broad-spectrum antibiotics. Crystal studies of the inhibitor bound to pyrH are ongoing for structure-based drug discovery. (This work presents detailed biological data, SAR analysis, and efficacy data in the target product profile table.) The knowledge obtained in this study provides valuable insights into the development of potential antibiotics against MRSA.

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Poster Presentation : **MEDI.P-394**

Medicinal Chemistry

Exhibition Hall 2 FRI 11:00~13:00

Diabetic Retinopathy: Exploring Innovative Transglutaminase 2 Inhibitors

Ga Young Park[*], **JIhee Kang**[1], **Jieon Lee**[1], **Jihoon Lee**[1], **Taeeun Kim**[1], **Hyeowon Seo**[1], **Minsoo Song**[1,*]

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Transglutaminase 2 is an enzyme that catalyzes the formation of protein crosslinks between glutamine and lysine residues through transamidation to create isopeptide bonds. Besides catalyzing cross-linking reactions, the transamidase activity of TGase2 plays an important role in various cellular processes such as differentiation, apoptosis, inflammation, cell migration and wound healing. Recently, TGase2 has been reported to be closely related to diabetic complications such as diabetic retinopathy, aortic insufficiency, lung metastasis, and chronic kidney disease, and is being targeted as a therapeutic target. TGase2 is expressed in ocular tissues such as the retina and lens and may be related to ophthalmic diseases such as cataract and glaucoma. In a related study, Ha’s group revealed that increased activity of TGase2 plays a central role in vascular endothelial growth factor (VEGF)-induced vascular leakage in diabetic retinopathy. Based on these concrete mechanistic rationale, we have been making efforts to develop a novel class of TGase2 inhibitors for diabetic retinopathy. We have discovered several small molecule inhibitors for TGase2 based on our in vitro assays (array-based on-chip assay and ZediXcite fluorescence assay). In situ cellular assays using human retinal endothelial cells (HRECs) showed potent inhibitory activities in dose-dependent fashion (IC50’s 90 and 70 nM for Compd 1 and 2, respectively). Both TGase2 inhibitor 2 showed complete inhibition of vascular leakage in STZ-induced diabetic retinopathy mouse model (i.p.). It was also found that the activation of TGase2 is the root cause of vascular leakage in diabetic retinopathy from our mechanistic study. However, pharmacokinetic properties of 1 and 2 both in vitro and in vivo revealed that there are some rooms to be improved. Our on-going efforts to develop a novel small molecule inhibitor for TGase2 for diabetic retinopathy are described here.

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Poster Presentation : **MAT.P-287**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Fixed bed column selective adsorption of 1-octene from binary liquid olefin/paraffin mixtures using ion-exchanged 13X zeolites

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1-octene, one of the linear alpha olefins, is used as a starting material in the petrochemical industry, such as surfactants and plasticizers. However, the major obstacle to obtain high-purity 1-octene is the separation and purification of 1-octene from 1-octene/*n*-octane mixture. In this study, the adsorptive separation of 1-octene from 1-octene/*n*-octane mixture has been investigated using ion-exchanged 13X zeolite adsorbents with different cations (Na^+, Li^+, Ca^{2+}, and K^+). Fixed bed column adsorption experiments have been conducted to determine the adsorption properties of ion-exchanged 13X zeolite adsorbents. The adsorption and desorption capacity of 1-octene for ion-exchanged 13X zeolites has been studied systematically as a function of cations and 1-octene fractions. In addition, the Thomas and Yoon-Nelson models were employed to the 1-octene breakthrough curves to elucidate the role of cations for the selective 1-octene adsorption.

Poster Presentation : **MAT.P-288**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Solvent Effects on the Light-stimulated Isomerization of Azobenzene Derivatives

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Two different azobenzene derivatives with long hexyloxy linkage: (1) HexOAz and (2) AzBuPy were synthesized. Their photoisomerization properties were conducted in different solvents on UV-visible absorption and fluorescence spectroscopy and 1H NMR spectroscopy. As the azobenzene derivatives possess light-induced reversible molecular structure changes from trans-to-cis and cis-to-trans by irradiation with UV and visible light, we examined the light-driven isomerization of synthesized azobenzene derivatives. Intriguingly, HexOAz showed solvent dependent photo-responsive properties; the non-polar solvents produced more cis-isomers (> 90%) than the polar solvents, which could be observed through spectroscopic measurements. Whereas AzBuPy had excellent photoisomerization performance in any solvents. In addition, the stable and repetitive monomer fluorescence switching was able to be investigated by varying UV and visible light irradiation. Moreover, the aggregates prepared from AzBuPy exhibited constant photoswitching up to ten cycles under different wavelengths of light illumination. Therefore, here, we reported the outstanding light-responsiveness of azobenzene derivatives in solvents and aggregate states and envisaged that would be useful in application of sensors and further optoelectronic research.

Poster Presentation : **MAT.P-289**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Molecular-Linked Z-Scheme Heterojunction of Ti^{3+}-Doped TiO_2 and WO_3 Nanoparticles for Photocatalytic Removal of Acetaldehyde.

Yeseul Hong, Hyoyoung Lee[1,*]

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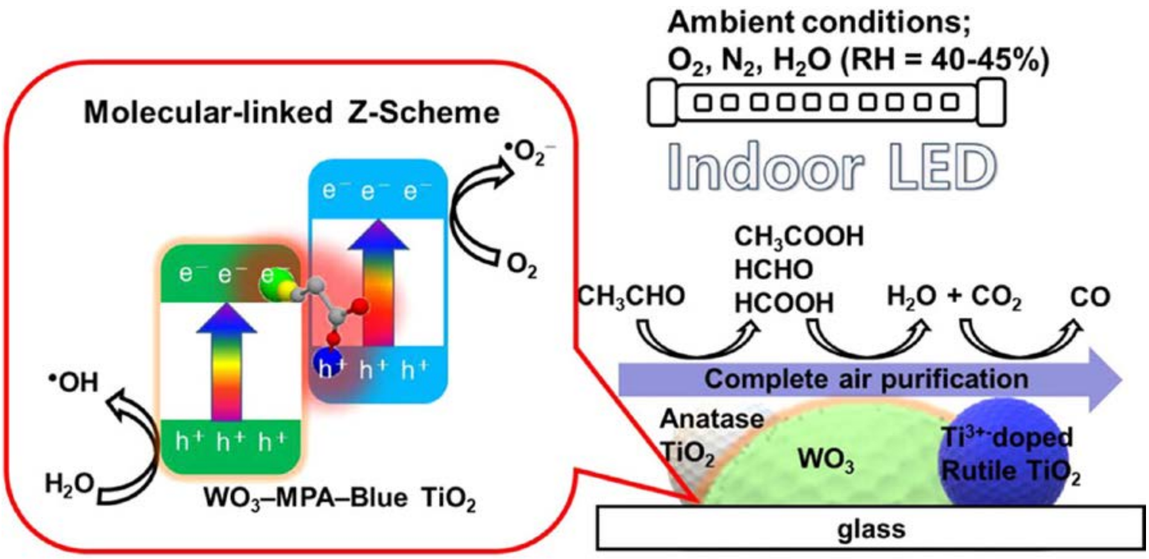
Photocatalytic removal of indoor organic air pollutants is effective, but there are practical limits to catalytic activation by indoor conditions. Here, we report a molecular-linked heterojunction of semiconducting metal oxide nanoparticles (e.g., Blue TiO_2 and WO_3) that can be activated by wide-range light including an indoor light-emitting diode (LED) under ambient conditions. Chemically reduced Blue TiO_2 improves visible light absorption of white TiO_2 by regulating the electronic structure with self-doping of Ti^{3+}. The heterojunction between Blue TiO_2 and WO_3 is formed via a molecular linker, and a hybridized electronic structure of a molecular-linked Z-scheme alignment is generated without changes in chemical characteristics, increasing utilization of indoor light and effectively improving electron–hole separation. WO_3 sufficiently adapts to the photooxidative degradation of air pollutants by $^{\bullet}OH$, while Blue TiO_2 leads to the effective generation of $^{\bullet}O^{2-}$, leading to the complete decomposition of gaseous acetaldehyde (CH_3CHO) to CO_2 and CO without remaining organic byproducts (e.g., formaldehyde). As a robust interfacial contact, molecular-linked heterojunctions provide efficient charge separation and highly stable performance and enhance solution-processable homogeneous coatings of metal oxide photocatalysts on real surfaces.


Ambient conditions;
O2, N2, H2O (RH = 40-45%)
Indoor LED
Molecular-linked Z-Scheme
•O2−
O2
e− e− e−
h+ h+ h+
•OH
H2O
WO3–MPA–Blue TiO2
CH3CHO
CH3COOH
HCHO
HCOOH
H2O + CO2
CO
Complete air purification
Anatase TiO2
WO3
Ti3+-doped Rutile TiO2
glass

Poster Presentation : **MAT.P-290**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Encapsulation of kojic acid within the gallery of layered yttrium hydroxide: Stability, release, and tyrosinase inhibition behavior

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Kojic acid (KA), known chemically as 5-Hydroxy-2-(hydroxymethyl)-4H-pyran-4-one, has garnered significant attention due to its diverse biological activities. It is widely employed in cosmetic products for skin lightening and as a food additive to prevent oxidative browning in fruits and vegetables. However, the effectiveness of KA is hindered by its susceptibility to pH and temperature fluctuations, as well as oxidation after exposure to UV light, necessitating improvements for practical applications. Organic/inorganic hybrid systems provide a relevant way to overcome these limitations by capitalizing on the unique advantages of both organic and inorganic substances, aiming to create synergistic effects. In our study, KA was intercalated into the interlayer space of layered yttrium hydroxide (LYH) through a two-step host-guest reaction involving dodecylsulfate and basic ethoxide anions. The resulting KA-LYH demonstrated significantly enhanced stability against light, heat, and oxygen compared to free KA. While KA-LYH exhibited minimal release of KA in saline solution and simulated seawater, it displayed sustained release of KA in a phosphate buffer solution. The cumulative KA release was best described by the parabolic diffusion model, often employed for processes with rapid initial-stage release. Importantly, the tyrosinase inhibition ability of KA remained essentially unchanged after release from the LYH gallery, showcasing the sustained effectiveness of KA-LYH in biological applications.

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Poster Presentation : **MAT.P-291**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Amphiprotic brush-grafted magnetic adsorbents: targeting hydrophilic and hydrophobic microplastics

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We explored the synthesis and properties of amphiprotic magnetic particles (AMPs) through sequential coatings. By adjusting hydrophobic content, hydrophilic, amphiprotic, and hydrophobic particles are formed, with optimal synthesis at a 71% hydrophilic to 29% hydrophobic ratio. These AMPs disperse well in oil/water mixtures, facilitated by polyethyleneimine (PEI) for hydrophilic microparticle (MP) removal and water dispersion, and octadecylamine (ODA) for hydrophobic MP elimination and oil dispersion. AMPs effectively remove both MP types in water and hydrophobic MPs in pure oil. The method is applicable for removing hydrophobic MPs in oil spills on water bodies.

Poster Presentation : **MAT.P-292**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Hybrid polymer-based air-filtering mask for respiratory protection

<u>Donggeon Lee</u>, Won san Choi*

Department of Chemical & Biological Engineering, Hanbat National University, Korea

Air-filtering masks, commonly referred to as respirators, shield wearers from inhaling particulate matters (PMs) in polluted air and airborne pathogens during events like the COVID-19 pandemic. The fibrous medium, serving as the filtration layer, stands as the paramount component of an air-filtering mask. This article introduces the Lego-stamping approach for synthesizing amphiprotic air-filtering masks. The removal efficiency, pressure drop, reuse rate, antibacterial ability, and mechanical properties of our mask manufactured using the Lego-stamping method were tested and ultimately compared to commercially available KF-94 masks.

Poster Presentation : **MAT.P-293**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhanced Lithium-Ion Battery Performance through Pseudocapacitance-Driven Lepidocrocite-Type Titanate/NiCo-LDH Heterojunction Engineering

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[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Since introducing the concept of secondary batteries decades ago, materials scientists have continuously pursued research into next-generation anode materials beyond graphite-based technologies. However, achieving stability and high energy density with a single material has proven challenging. Recently, research into functional composites utilizing electrostatic attraction and van der Waals forces has gained momentum as a solution to these challenges. To maximize the synergistic effects of each component in these composites and minimize the trade-offs of incorporating high-energy-density components, we present a study of partial phase transitions in layered materials based on intercalation to form a large number of grain boundaries and maximize the performance of diffusion-independent surface electron storage at nanointerfaces. To maximize the surface charge storage reaction beyond the crystallographic theoretical capacity, heterojunctions composed of chemically exfoliated transition metal oxide nanosheets (Lepidocrocite-Type Titanate and Nickel-Cobalt Layered Double Hydroxide) are synthesized, and the phase transition process is controlled to induce the formation of various polymorphs. As a result, the crystal mismatch of the transition metal oxide nanoparticles derived from the two-dimensional nanosheets promoted the formation of more grain boundaries and provided surface storage sites accessible to Li-ions.

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Poster Presentation : **MAT.P-294**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

MOF-Derived Cu_2S/N-Doped Carbon on Titanoniobate Hollow Spheres for High-Performance Sodium Storage

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Efforts to develop cost-effective sodium-ion batteries as a potential next-generation alternative to address the resource scarcity and high costs of lithium-ion batteries are actively underway. To improve the performance and stability of sodium-ion batteries, it is necessary to create new anode materials that can accommodate the greater size and slower mobility of Na-ions in comparison to Li-ions. This paper presents a new hybrid anode material named Cu_2S/NC/TN-HS, synthesized by MOF-derived Cu_2S/N-doped carbon layers on titanoniobate hollow spheres. This synthetic methodology encompasses the structural evolution of the carbon framework through the pyrolysis of Cu-MOF and the conversion of exposed metal ions into electrochemically active species via a sulfuration reaction. The structural features and improved electrochemical properties of Cu_2S/NC/TN-HS were confirmed by using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and X-ray diffraction analysis. The study shows that Cu_2S/NC/TN-HS has better cycling performance due to enhanced ionic and electronic conductivity and structural stability compared to other titanoniobate-based anode materials, indicating its potential for a highly efficient sodium storage.

Poster Presentation : **MAT.P-295**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Design of Vertically Aligned Ultrathin MoS_2 Nanosheets on Two-Dimensional Covalent Organic Nanosheet Hollow Spheres with Multiple Redox Sites for Enhanced Sodium Storage Performance

Jimin Kim, **Seung-Min Paek**[*]

Department of Chemistry, Kyungpook National University, Korea

The demand for secondary batteries has significantly increased due to the widespread use of electric vehicles and huge energy storage systems, unlike the past when mobile devices were the primary focus. Sodium-ion batteries have attracted research interest as a new energy storage technology due to the abundance of sodium compared to limited and expensive lithium resources. MoS_2, due to its large interlayer spacing, has a high reversible capacity for Na-ions, making it a potential anode material for sodium-ion batteries. However, its low ionic/electrical conductivity, along with large volume changes during charge/discharge cycles, cause active material loss, decreased conductivity, and capacity decrease, ultimately reducing battery durability. This research utilized a hydrothermal synthesis method to promote the vertical growth of MoS_2 on Covalent Organic Nanosheets (CON) substrates. This approach reduced the diffusion distance for Na-ions and increased the number of active sites, leading to improved electrical conductivity of MoS_2. As a result, the electrode durability and performance were significantly enhanced. The synthesized CON@MoS_2-HS demonstrated better capacity performance than recently reported MoS_2-based anode materials. This structural design technique is anticipated to greatly help reduce volume expansion, boost structural stability, and enhance the ionic/electrical conductivity of electrode materials, thus boosting the performance of sodium-ion batteries.

Poster Presentation : **MAT.P-296**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Nanoarchitectural Engineering for Enhanced Lithium and Sodium Storage Performance of Iron-Doped Layered Titanium Oxide-Derived Pseudobrookite

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Sodium is more abundant on Earth than lithium, which makes sodium-ion batteries (SIBs) an attractive substitute for lithium-ion batteries (LIBs). The large ion radius and slow kinetics of sodium ions limit the use of graphite-based anode materials. Research has focused on titanium oxide (TiO_2) as an alternative to graphite because of its structural stability, cost effectiveness, and sustainable properties. However, the low conductivity of TiO_2 is still a major obstacle. Metal doping is recognized as an efficient technique for improving electrochemical performance by optimizing the inherent electrical structure of materials. We synthesized iron-doped layered titanium oxides hollow spheres (FTO HSs) using nanosheets of $Fe_{0.8}Ti_{1.2}O_4$ (FTO NSs) by the layer-by-layer (LBL) self-assembly technique. The crystal structure was verified by XRD and HR-TEM analysis, and the diffraction peaks were identified as belonging to the pseudobrookite structure of Fe_2TiO_5. FTO HSs can improve ion diffusion from an electrochemical perspective because of their large surface area of the hollow spheres. Galvanostatic charge/discharge cycling shows that FTO HSs have a higher reversible capacity compared to TiO_2 HSs in the control group.

Poster Presentation : **MAT.P-297**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Unveiling the Electrochemical Behaviors of Aqueous Zinc-Ion Batteries: X-ray Absorption Fine Structure Study

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Various next-generation batteries are being developed, and we are exploring about aqueous zinc ion battery (AZIB), which attracting attention as the next-generation battery due to outstanding safety and cost competitive advantage. There have been a variety of cathode materials utilized. Manganese dioxide (MnO2) has been addressed by prior studies that Zn2+ can be inserted into crystal structure because it exhibits several crystal structures with tunnel-type or layer-type structure. To construct a [MnO6] octahedral unit, each Mn4+ ion is precisely surrounded by six oxygen neighbors, and these units are connected by the edges and/or corners. Understanding the energy storage mechanisms is essential for the one-step evolution of cathode materials for AZIB. Polymorphs significantly affect the electrochemical reaction, thus involving complex reaction mechanisms. X-ray absorption fine structure (XAFS) is a powerful technique used for the analysis of nanostructured materials, widely used in the field of battery research. It involves the measurement of the absorption of X-ray by the material, which can provide information about oxidation state, chemical bonding of the materials and the local geometry structure during charge/discharge process. The oxidation state changes could be quantitatively estimated by edge energy analysis by comparing the reference MnO2 and Mn2O3 samples. It was also possible to unveil further about the reaction mechanism at each voltage by examining the structural change in the local geometry of [MnO6] unit through a careful analysis of pre-edge region and EXAFS spectra. These findings contribute to further understanding of the reaction mechanisms and capacity fading phenomenon and suggest practical strategies for next-generation zinc-ion batteries.

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Poster Presentation : **MAT.P-298**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

The application of uncomplicated thermal treated molybdenum silicide as anode for lithium-ion batteries

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Considerable researches have been devoted to the study of lithium-ion batteries (LiBs) in the past decades due to their high theoretical capacity and other properties, which like high charge retention, high volumetric and gravimetric specific energy, to be a high-performance LiB option. Metal silicides have advantageous features compared to other silicon-based anode materials, which are maintaining nano-structure during electrochemical reaction because of their high stability. In this study, we treated metal silicides under various temperatures and atmospheres. We characterized all samples by XRD, N2 adsorption & desorption, scanning electron microscope and electrochemical tests. Among them, molybdenum silicide (MoSi2) shows a remarkable transition. There were substantial structural and chemical transition throughout the calcination in air. And these transitions provoked compelling electrochemical improvements in reversible capacity and cycle retention.

Poster Presentation : **MAT.P-299**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Hybridization with conductive multimetallic oxide nanosheets to boost the electrocatalytic activity

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[1]*Department of Applied Chemistry, University of Seoul, Korea*

Hybridization with conductive 2D nanosheets has evoked intense research activities because of its usefulness in optimizing the electrocatalytic activities of nanostructured materials. To circumvent the limited hybridization impact and high price of graphene and RuO_2 nanosheets, we synthesize noble-metal-free conductive multimetallic oxide nanosheets as economically-feasible efficient hybridization matrices via the fine-control of chemical composition and defect structure. The diversification of cationic composition of multimetallic oxide nanosheets enables to finely tailor anion vacancy and surface bond polarity, leading to a strong interfacial electronic coupling with hybridized species and an improvement of charge/mass transfer. The composition-controlled multimetallic oxide nanosheets can function as emerging hybridization matrices for enhancing electrocatalytic oxygen evolution activity of hybridized species. The universal validity of these nanosheets is further corroborated by the hybridization-induced improvement of visible light photocatalytic activity of hybridized semiconductors. The present study highlights the high efficacy of hybridization with surface-optimized multimetallic oxide nanosheets in exploring efficient hybrid electrocatalysts/photocatalysts.

Poster Presentation : **MAT.P-300**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Interface engineering approach to optimize the electronic coupling and electrocatalyst performance of layered double hydroxide

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[1]*Department of Applied Chemistry, University of Seoul, Korea*

An interface engineering has attracted intense research efforts because of its usefulness in optimizing various catalytic activities of nanostructured materials. Herein we developed an interface engineering route to explore high-performance hybrid electrocatalysts by introducing holey TiN nanolayer as buffer layers. Multiscale hybrid electrocatalysts of Ti foam@holey TiN-Ni-Fe-layered double hydroxide (LDH) were synthesized by sequential oxidation-nitridation of Ti foam, which was followed by the crystal growth of LDH. The obtained Ti@holey-TiN-LDH nanohybrid displayed an outstanding performance as an oxygen evolution electrocatalyst with very low overpotential of ~246 mV at 50 mA cm^{-2} in simulated seawater media. Combined spectroscopic analyses confirm the pivotal role of holey TiN buffer layers in enhancing interfacial electronic coupling between LDH and Ti foam, resulting in the robust electrical connection between LDH and Ti metal substrate. The benefit of hierarchical hybrid structure on the electrocatalyst functionality can be ascribed to the provision of many electrochemical active sites and the enhancement in charge/mass transfer properties.

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Poster Presentation : **MAT.P-301**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

One-pot nitridation-exsolution route to high-performance metal nanocluster-metal nitride electrocatalysts

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Exsolution has garnered significant research interest because of its high efficacy in synthesizing metal nanocluster-based composite electrocatalysis. In this study, we report a rationally designed single-step nitridation-exsolution synthetic route to high-performance hydrogen evolution reaction (HER) electrocatalyst. The NH_3 treatment of Ru-substituted oxide nanowires at evaluated temperature induces the exsolution of Ru nanoclusters and also the phase transition to holey metal nitride nanotubes. The obtained Ru exsolved metal nitride nanotube exhibits much higher HER electrocatalytic activity than that of Ru deposited homolog, highlighting the benefit of the nitridation-exsolution approach. The crucial effect of simultaneous nitridation-exsolution process on the HER electrocatalytic activity is attributable to the improved charge transfer kinetics, increased porosity, and the increase of electrocatalytic kinetics. The present study demonstrates that the single-step nitridation-exsolution synthetic strategy can provide an effective means to explore robust composite electrocatalyst materials.

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Poster Presentation : **MAT.P-302**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Strongly-coupled layered double hydroxide-RuO_2 nanohybrids with efficient photocatalytic nitrogen fixation activity

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Department of Materials Science and Engineering, Yonsei University, Korea

Hybridization with conductive nanostructures has evoked great deal of research activity owing to its high efficacy in improving the photocatalyst functionality of hybridized semiconductors. Herein we synthesize highly efficient and stable hybrid photocatalysts via the reinforcement of electrostatic interfacial interaction between hybridized nanosheet species. The electrostatically-driven self-assembly between Cu-Cr-layered double hydroxide (Cu-Cr-LDH) nanosheets and conductive RuO_2 nanosheets yields strongly-coupled hybrid materials with excellent visible-light-driven photocatalyst functionality for N_2 fixation. The hybridization of Cu-Cr-LDH with RuO_2 nanosheets leads to the enhancement of light absorption ability, the decrease of electron-hole recombination rate, and the increase of surface area. The improved photocatalytic activity of LDH-RuO_2 nanohybrids can be attributed to the strong interfacial electronic coupling between Cu-Cr-LDH and RuO_2 nanosheets, resulting in the optimization of optical and electronic properties. This study clearly demonstrates that the exfoliated RuO_2 nanosheets can act as effective hybridization matrices to improve the photocatalytic nitrogen fixation activity of inorganic nanosheets.

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Poster Presentation : **MAT.P-303**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Seed-Mediated Synthesis of colloidal Zn3P2 Quantum dots

Ju Ho Kim, Jiwon Bang*

Dept. of Chemistry, Incheon National University, Korea

Colloidal Quantum dots (QDs) present a significant potential for advancing various light-based technologies, including displays, solid-state lighting, photovoltaics, photocatalysis, and biological imaging, due to their unique light absorption and emission properties. Among these materials, colloidal nanocrystals based on Zinc phosphide (Zn3P2) emerge as a particularly promising optoelectronic material. This is attributed to their nearly ideal direct optical bandgap of 1.5 eV, high optical absorption coefficient, extensive minority-carrier diffusion lengths, and capability to emit across the full visible spectrum by modulating their size and shapes. Despite these advantages, the synthesis of Zn3P2 QDs has faced challenges, primarily due to the low formation enthalpy of the Zn3P2 crystal and the stability of Zn-P molecular species, which complicates the crystalline growth of Zn3P2 QDs, leading to a scarcity of reports on Zn3P2 QDs with well-defined optical properties. In here, we introduce a novel synthesis protocol for Zn3P2 QDs, leveraging InP cluster seeds to initiate the formation of the Zn3P2 crystalline lattice. The utilization of InP cluster seeds with a pseudo zinc-blended structure facilitates the cubic phase growth of Zn3P2 crystals. The resulting Zn3P2 QDs demonstrate a clear band edge absorption peak and are emissive under ambient conditions. Furthermore, applying a ZnS shell to the Zn3P2 QDs significantly enhances their photoluminescence. The innovative approach of using InP cluster seeds not only promotes the crystalline growth of Zn3P2 QDs but also yields QDs with exceptional optical properties, marking a significant advancement in the field of optoelectronics.

Poster Presentation : **MAT.P-304**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

The combination of cetyltrimethyl ammonium cations (CTA$^+$) and Br$^-$ for Cu bottom-up filling at Through-Silicon Vias (TSVs)

Hui Won Eom, HaeJin Kwak, Myung Jun Kim[*]

School of Chemical Engineering, Sungkyunkwan University, Korea

The advancement of semiconductor packaging relies heavily on the vertical stacking of chips, necessitating copper wiring with superior electrical conductivity and reliability. Notably, Through-Silicon Via (TSV) technology emerges as a pivotal method for facilitating interconnections in cutting-edge packaging designs. After creating high-aspect-ratio TSVs, Cu electrodeposition is performed to achieve defect-free Cu interconnection. To this end, copper electrodeposition becomes instrumental, demanding a meticulous bottom-up filling process that circumvents deposition flaws at TSV entrances and sidewalls while effectively promoting deposition at the base. This bottom-up filling is achievable through the introduction of specific organic additives into the electrolyte. Existing literature predominantly discusses the effectiveness of three-additive combinations (suppressors, accelerators, and levelers) or single suppressors in enabling Cu bottom-up filling. Various studies explore the use of ammonium-functionalized levelers, polymeric suppressors, and accelerators within three-additive systems. Additionally, halide ions such as bromide and iodide have been identified as effective levelers for inducing bottom-up filling at TSVs. One notable single-additive method utilizes Tetronic 701, leveraging its S-shaped negative differential resistance (S-NDR) behavior. This study delves into the impact of cetyltrimethylammonium cation (CTA$^+$) and bromide ions on TSV filling in electrolytes devoid of polymeric suppressors. Electrochemical analysis elucidates the adsorption dynamics of CTA$^+$ and Br$^-$ on the substrate, facilitating adjustments to their concentrations to foster bottom-up filling. This presentation outlines the electrochemical behavior of each additive, TSV filling outcomes relative to additive concentration, and the underlying filling mechanism under optimized conditions.

Poster Presentation : **MAT.P-305**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Surface Morphology Control in Sn-Bi Electrodeposition through Additive Utilization

<u>Yoojin Hwang</u>, Jeong Ho Lee, Myung Jun Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

In semiconductor packaging technology, establishing robust electrical connections between chips is crucial for manufacturing high-performance electronic devices. Microbumps and low-temperature solders are currently favored for their ability to enhance electronics integration compared to traditional Au wiring processes. The microbumps are typically composed of Cu due to its low electrical resistivity, while Sn-Ag is widely utilized as solder material. However, conventional thermo-compression (TC) bonding with Cu pillars and Sn-Ag solder, typically conducted at around 250℃, poses reliability issues in bonding process. High temperatures during bonding can cause wafer warpage due to differences in the thermal expansion coefficients between the top and bottom of bonding wafers, resulting in misalignment and defects. This issue significantly reduces process yield and electronic performance. Thus, reducing bonding temperature is imperative by adopting solder materials with lower melting temperatures, such as Sn-Bi. Sn-58 wt% Bi offers a promising melting temperature of approximately 139℃. However, the electrodeposition process for Sn-Bi is less mature compared to Sn-Ag. To prevent defects at the bonding interphase, it is crucial to develop an electrodeposition method that produces smooth Sn-Bi films. This study investigates the effects of additives on controlling the surface morphology of Sn-Bi films, exploring the impact of electrolyte composition, current density, and the type and concentration of additives on Sn-Bi electrodeposition.

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Poster Presentation : **MAT.P-306**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Utilizing Additives in Cu Electrodeposition for Twin Structure Development

Jeong Ho Lee, Yoojin Hwang, Myung Jun Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

In current semiconductor 3D packaging, thermo-compression bonding technology utilizing Cu microbumps and Sn-Ag solder is employed for electrically connecting chips. However, the pitch of microbumps will be limited to 10-20 μm due to the lateral expansion of solder during the bonding process, restricting further enhancement of interconnection density and electronic performance. To address this limitation, hybrid bonding technology has emerged, which is based on the direct bonding between Cu-Cu or insulators (such as SiO2, SiCN, or polymers), significantly increasing interconnection density. Nevertheless, conventional Cu-Cu direct bonding methods suffer from drawbacks such as high temperature, pressure requirements, and lengthy bonding times. Elevated temperatures can cause wafer warpage, adversely affecting bonding reliability. Recent research has proposed a solution by utilizing Cu with twin structures to lower bonding temperatures, presenting a promising avenue for low-temperature hybrid bonding processes. Thus, precise control over the twin structure through Cu electrodeposition methods becomes imperative for advancing such processes. This study delves into the effects of additives on controlling the microstructure of Cu films formed via electrodeposition. It examines how varying electrodeposition parameters and additive types/concentrations influence Cu microstructures during electrodeposition. Based on the findings, optimal molecular structures and electrodeposition conditions for achieving twin structures will be proposed.

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Poster Presentation : **MAT.P-307**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Improving Zn Anode Stability in Zn Ion Batteries by Benzene-Based Additives for Prolonged Lifespan

Hana Lim, Jiwoo Oh, Myung Jun Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

Lithium-ion batteries (LIBs) are indispensable components in electrical energy storage systems, powering portable electronics and electric vehicles. However, their reliance on flammable organic solvents renders them potentially hazardous. Consequently, there has been a significant research effort to develop safer alternatives, including aqueous metal-ion batteries, with Zn ion batteries (ZIBs) being a prominent example. Compared to conventional LIBs, ZIBs offer cost-effectiveness, safety, and environmental friendliness. Nonetheless, the practical application of aqueous Zn ion batteries (AZIBs) is hindered by their relatively short lifespan. The use of Zn foils as negative electrodes in AZIBs presents challenges such as dendrite growth, corrosion, and hydrogen evolution reaction (HER), with dendritic growth posing a particularly severe risk of short circuits between electrodes. Various strategies have been proposed to address these limitations, including surface-coating-layer modifications of Zn anodes, separator design enhancements, and electrolyte modulation. Among these, optimizing the electrolyte using additives stands out as a simple and economical approach. In this study, we investigated the use of benzene-based additives to enhance the cycle performance of AZIBs. Our results demonstrate that with the optimized benzene-based additive, Zn-Zn symmetric cells achieved a cycle life of over 3,500 hours at 1 mA/cm² and 1 mAh/cm², and 1,000 hours at 5 mA/cm² and 5 mAh/cm². This presentation will delve into the relationship between the molecular structure of benzene-based additives and their effectiveness in controlling Zn morphology, highlighting how the optimized additive significantly extends the lifespan of Zn negative electrodes.

Poster Presentation : **MAT.P-308**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Electrochemical Investigation on How CTA$^+$, Br$^-$, and Ag$^+$ Affect Anisotropic Growth of Gold Nanorods

Yujin Min, Seolim Yoon, Myung Jun Kim*

School of Chemical Engineering, Sungkyunkwan University, Korea

Gold nanorods (AuNRs) are highly versatile plasmonic nanoparticles with wide-ranging applications in sensing, therapeutics, photocatalysis, and optoelectronics, owing to their adjustable plasmonic properties across the visible and near-infrared spectrum. The plasmonic and photocatalytic behaviors of AuNRs are intricately tied to their aspect ratio, defined as the ratio of length to width. Consequently, extensive research has focused on synthetic methods to precisely control the aspect ratio of AuNRs. While seed-mediated growth methods have been predominantly employed for AuNR synthesis, approaches involving Ag$^+$ have emerged as convenient means to enhance yield and uniformity. Despite these advancements, the underlying mechanism governing the anisotropic growth of AuNRs remains elusive. Previous discussions on the growth mechanism have been limited, often relying solely on synthetic results. Consequently, existing mechanisms may fail to fully explain aspect ratio changes under varying chemical environments during AuNR growth. This study investigates the effects of CTA$^+$, Br$^-$, and Ag$^+$ on the anisotropic growth of AuNRs. Electrochemical analyses shed light on the influence of Ag$^+$ on the adsorption behavior of Br$^-$ and CTA$^+$. Notably, silver preferentially adsorbs on the sides in the presence of CTA$^+$ ions. The presentation will provide detailed insights into the impact of each additive on Au reduction dynamics and the formation of suppression layers on AuNRs across varying adsorption durations. Furthermore, this presentation will explore how these adsorbates contribute to alterations in the aspect ratio of AuNRs. These findings hold potential to inform refinements in synthetic methodologies, thereby broadening the scope of AuNR applications.

Poster Presentation : **MAT.P-309**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Oxygen Vacancy Generation and Stabilization in Layered Double Hydroxide Nanosheets for a Highly Efficient Oxygen Evolution Reaction

Birhanu Bayissa Gicha, **Jaebeom Lee**[1,*]

1Research Institute of Materials Chemistry, Chungnam National University, Korea

[1]Chemistry, Chungnam National University, Korea

Oxygen vacancy (Vo) is ubiquitous, playing a critical role in tuning the electronic configuration and optimizing the adsorption of adsorbates in the OER process. However, fine control over the density and stabilization of Vo is a big challenge in the highly oxidizing environment of OER. Herein, we have fabricated bulk NiFeCo LDHs via the hydrothermal method and exfoliated them into thin sheets rich with Vo using high-energy Ar-plasma. We doped fluoride to simultaneously modulate the charge distribution of surrounding atoms and stabilize Vo by taking advantage of the extremely high electronegativity and similar ion diameter to oxygen of fluoride. The material had excellent OER activity, with a low overpotential of 200 mV at 10 mA cm-2 and a Tafel slope of 34.6 mV dec-1. DFT calculations support the claim that Vo and fluoride substantially increase NiFeCo LDH OER activity by modifying the electronic structures of the catalytically active sites.

Poster Presentation : **MAT.P-310**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Control of water infiltration into voids within dry bottom ash (dBA) by polymer coating

In Soo Koo, Yong Hun Jeon, Seog Woo Rhee[*]

Department of Chemistry, Kongju National University, Korea

In this study, we developed a method to control water infiltration into dry bottom ash (dBA) internal voids by coating the dBA surface with a polymer. Dry bottom ashes with an average particle size of approximately 5 mm were immersed in 0.1-10% poly(vinyl alcohol) aqueous solutions and coated with viscous polymer materials on the particle surface. The 1 g of sample completely dried at 110°C was added to 50 mL distilled water and allowed to infiltrate the water. The amount of water absorbed by the sample after a given time was measured using isothermal TGA method. In the untreated sample, about 20% of water was infiltrated based on the mass of dBA, while less than 5% of water was infiltrated in PVA-coated dBA under the same conditions. In conclusion, dBA coated with polymer maintains its light-weight material properties and it may be able to improve the disadvantage of general dBA, which absorbs a lot of water during the aging process of concrete.

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Poster Presentation : **MAT.P-311**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Characterization of composite materials synthesized from dry bottom ash and calcium carbonate

<u>Yong Hun Jeon</u>, In Soo Koo, Seog Woo Rhee[*]

Department of Chemistry, Kongju National University, Korea

In this study, we synthesized and characterized composite materials using dry bottom ash (dBA) and calcium carbonate. Dry bottom ashes with an average particle size of approximately 5 mm were immersed in poly(vinyl alcohol) (PVA) aqueous solutions and coated with viscous polymer materials on the particle surface. Spherical composite materials were prepared by mixing dBA particles coated with adhesive PVA and calcium carbonate nanoparticles to fill the surface voids of dBA. The crystal structures of the synthesized composite materials were analyzed using powder XRD, the chemical compositions were analyzed using WD–XRF, and the thermal decompositions of calcium carbonates were analyzed using TGA. SEM images showed that the voids on the surface of dBA in the composites were filled with calcium carbonates. In conclusion, dBA composites modified with polymers and inorganic materials have the potential to be used as light-weight materials in the construction field.

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Poster Presentation : **MAT.P-312**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Synthesis of copper-imidazole coordination compounds and evaluation of their insecticidal activities against termites

Choungwon Shin, Jinkwon Kim[1,*], Seog Woo Rhee[1,*]

Depratment of Chemistry, Kongju National University, Korea
[1]*Department of Chemistry, Kongju National University, Korea*

In this study, we synthesized imidazole-based copper coordination compounds and investigated their activities as termite inhibitors. Copper-imidazole coordination compounds were synthesized by the reaction of Cu^{2+} ions and imidazole ligands in ethanolic solutions. Functional groups were analyzed using FT-IR spectroscopy, chemical compositions were analyzed using elemental analyzer, and Cu^{2+} coordination environments were analyzed using UV-Vis spectroscopy. In no-choice tests on wood blocks treated with aqueous solutions of copper-imidazole coordination compounds at concentrations greater than 0.05%, all termites died within 28 days, resulting in a 100% mortality. In conclusion, copper-imidazole coordination compounds showed activity as highly effective anti-termite agents.

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Poster Presentation : **MAT.P-313**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Surface modification of hydroxyapatite by dye and investigation of dye release in aqueous solution

Sung Ju Oh, Jinkwon Kim*, Seog Woo Rhee*

Department of Chemistry, Kongju National University, Korea

In this study, we investigated controlled dye release from aqueous dispersions of dye-modified hydroxyapatite. Hydroxyapatite was synthesized by the reaction of Ca^{2+} and HPO_4^{2-} under basic conditions. Amine groups were introduced to the surface of the hydroxyapatite particles using o-phosphorylethanolamine (PEA). Dye-conjugated hydroxyapatite (HAp-dye) was synthesized by the condensation reactions of the surface amines, glutaraldehydes, and dyes containing amine groups. The properties of the synthesized solid materials were characterized using FT-IR, XRD, SEM, and particle size analyzer. Desorption isotherms of the dyes were obtained by measuring the absorbance of the dye released from HAp-dye dispersed in buffer solutions (pH 6.0-8.0). Finally, a mechanism to explain the release of drugs immobilized on solid surfaces was proposed.

Poster Presentation : **MAT.P-314**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Halide Ion Mobility in Paired 2D Halide Perovskites : Ruddlesden-Popper Versus Dion-Jacobson Phases

Seonhong Min, Junsang Cho[1,*]

School of Chemistry and Energy, Sungshin University, Korea
[1]*School of Chemistry and Energy, Sungshin Women's University, Korea*

2D lead halide perovskites with tunable optoelectronic properties through modulating inorganic components and organic spacer ligands represent a promising candidate in perovskite optoelectronics. However, an intrinsic soft lattice of perovskites gives rise to a vacancy-mediated halide ion migration, which further affects the long-term stability of materials as well as devices. Here, halide ion mobility is evaluated using two different 2D perovskites yielded with butylammonium (BA) for the Ruddlesden–Popper (RP) phase and butane-1,4-diamine (BDA) for the Dion–Jacobson (DJ) phase, respectively. By probing the halide ion migration kinetics in the physically paired 2D bromide and iodide perovskite films, the softer lattice (RP) shows a lower activation energy of 50.9 kJ mol^{-1} as compared to that of more rigid lattice (DJ) of 60.8 kJ mol^{-1}. Given similar halide diffusion pathlength and halide mixing chemical potential, the binding mode (RP and DJ) can indeed dictate the overall halide ion stability. Understanding such halide ion mobility is important in designing perovskites with increased stability and performances at material and device levels.

Poster Presentation : **MAT.P-315**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Cyclic Metal/Metal-Oxide Conversion of Nanocrystals Array within 2D-Nanogap for High Performance Lithium-Ion Battery Anodes

Yu-Rim Hong, Jeong Sang Oh, In Su Lee[*]

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

Optimizing late transition-metal oxides at the nanoscale to enhance the reversible lithiation/delithiation mechanism, while gaining a profound understanding of nanocrystal (NC) conversion chemistry, holds significant importance for advancing next-generation lithium-ion battery (LIB) technologies. In this study, we focus on 1 nm-thin nanosheets of Ni_3CoO_x (referred to as 1 nm-NCO) synthesized via isomorphic transformation of NiCo layered double hydroxides within a two-dimensional (2D)-SiO_2 envelope. The ability of metal/metal-oxide NCs to undergo interconversion under redox-switching thermal treatment while maintaining reversibility served as inspiration for achieving similar outcomes under the demanding operational conditions of LIB redox cycles, employing the thin-NCO-defined 2D nanospace. Throughout charge/discharge cycles, the presence of an in situ formed solid-electrolyte-interphase layer on 1 nm-NCO facilitates fully reversible interconversion between reactive NC redox pairs. This is evidenced by comprehensive morphological and electrochemical analyses, leading to remarkable high-rate capability, with a specific capacity achieving 61.2% at 5.0 C compared to 0.2 C. Additionally, outstanding cycle stability is achieved, delivering a reversible capacity of 1169 mAh g^{-1} and 913 mAh g^{-1} with high average Coulombic efficiency (>99.2%) at 3.0 and 5.0 C for 1000 cycles, respectively. These achievements surpass those observed with other transition-metal oxides. The nanospace-confinement effect, observed to sustain reactive NCs and promote highly reversible conversion reactions during fast charging in LIBs, is particularly notable within the slit-like ultrathin 2D nanogap provided by 1 nm-NCO. In contrast, relatively thicker 7 nm-NCO anodes, with larger available space, demonstrate poor reversibility of NCs and inadequate cyclic stability under potential high-power density LIB applications.

Poster Presentation : **MAT.P-316**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

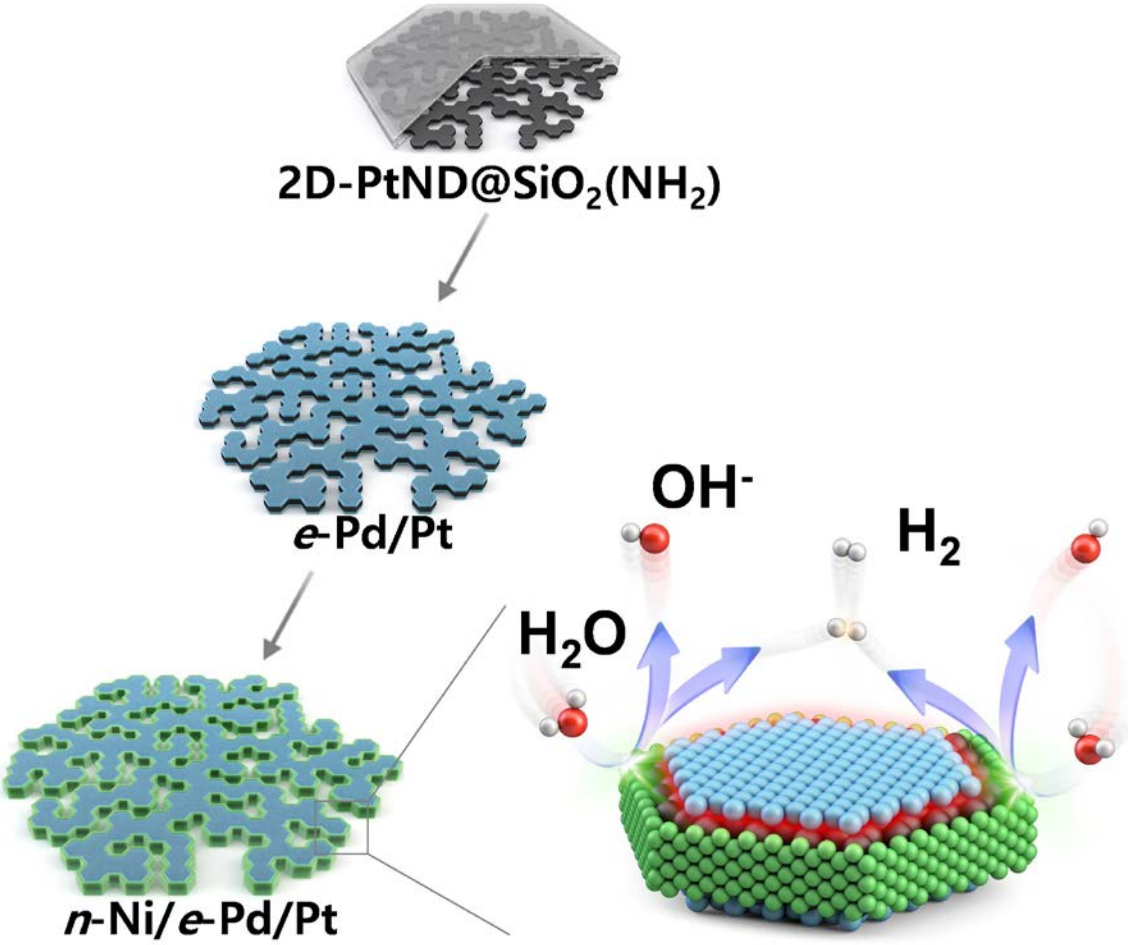
Formation and combining heterointerfaces on 2D Pt nanocrystals with tunable spatio- and facet- selective wet-chemical process

Byeongsu Gu, Kyeong-bin Kang[1], In Su Lee*

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

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

Maximizing the efficiency of nanocrystal (NC) catalysts involves strategically incorporating carefully designed interfaces formed by modifying specific facets and spatial arrangements with other materials of desired dimensions. However, creating these interfaces with precision using a sophisticated process presents significant challenges. Moreover, even slight variations in dimensions can lead to unforeseen issues such as obstruction of active sites, decreased accessibility, and reduced activity.In this study, we employed a wet chemical approach to precisely deposit Pd and Ni onto the available surfaces of porous 2D-Pt nanodendrites (NDs). By utilizing 2D silica nanoreactors to encase the 2D-PtND, we achieved the formation of an exclusively 0.5-nm-thick epitaxial Pd or Ni layer (e-Pd or e-Ni) on the flat {110} surface of 2D-Pt, while a non-epitaxial Pd or Ni layer (n-Pd or n-Ni) was typically deposited at the {111/100} edge in the absence of a nanoreactor. Significantly, these Pd/Pt and Ni/Pt heterointerfaces located at different positions exhibited distinct electrocatalytic performance due to variations in their interactions based on facet and location.After gaining a thorough understanding of facet- and spatio-specific interactions at the heterointerfaces, we realized the potential of combining different heterointerfaces within a single nanocrystal to achieve the desired structure for electrocatalysis. Consequently, by assembling these diverse and valuable heterointerfaces in the optimal 2D n-Ni/e-Pd/Pt catalyst, we successfully addressed the sluggish alkaline HER kinetics, resulting in a catalytic activity 7.9 times higher than that of commercial Pt/C.


2D-PtND@SiO$_2$(NH$_2$)
e-Pd/Pt
n-Ni/*e*-Pd/Pt
OH$^-$
H$_2$
H$_2$O

Poster Presentation : **MAT.P-317**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Investigating Colorimetric Assay Challenges: Reaction Pathways and Potential Pitfalls with Signaling Agents with Catalytic Gold Nanoparticles

Sang-Won Kim, Jae-Seung Lee*

Department of Materials Science and Engineering, Korea University, Korea

The investigation of colorimetric assays shows that o-phenylenediamine (OPD), a commonly used signaling agent, undergoes complex oxidation processes resulting in both dimerized and polymerized forms. The polymerized form affects the signal clarity of the assay. This study emphasizes the intricate behavior of gold nanoparticle-catalyzed OPD oxidation, which causes unusual signal variations. Polymerized OPD molecules were identified as the cause of signal disruptions through extensive spectroscopic and microscopic analysis. To enhance assay reliability, we modified assay conditions and introduced sodium nitrate as an alternative to sodium chloride, showcasing the intricate balance between reaction conditions and signal fidelity in colorimetric DNA detection.

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Poster Presentation : **MAT.P-318**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Selection of a Machine Learning Algorithm Appropriate for the Characteristics of OPV Data for Efficiency Prediction

Juyeon Hong, Hyojin Ban, Dongwook Kim*

Chemical Data-Driven Research Center, Korea Research Institute of Chemical Technology, Korea

Advances in computer science have enabled the efficient synthesis and optimization of materials, thus reducing the time required to evaluate compounds through experiments. We developed a platform for the systematic collection of Organic Photovoltaic (OPV) data and utilized the accumulated dataset for machine learning. Prediction performance was enhanced by creating features that consider the chemical structure and electronic states. To select the algorithms most suitable for this study, we compared the performance of four algorithms: XGBoost, Random Forest, Supprot Vector Machine, and Neural Network. The XGB model, which exhibited the highest performance with an R2 of 0.85, was used to predict physical properties (PCE, Jsc, Voc, FF).

Poster Presentation : **MAT.P-319**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

OPV Machine Learning with Molecular Fragment-based features

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Korea Research Institute of Chemical Technology, Korea

Organic photovoltaics(OPVs) is promising research field among renewable energies because of low costs and increased efficiency. The aim of this research is to select features for predicting the efficiency of OPVs and to improve the prediction of Power Conversion Efficiency (PCE) using machine learning. We selected donors and non-fullerene acceptors and performed fragmentation of molecular structures. The donor was divided into the backbone and side chain, while the acceptors were split into the ring, π-bridge, and end-group. This approach enables the generation of various features beyond device information and facilitates the handling of large molecules. We used XGBoost as prediction algorithm and validated an improvement in the test R-squared value from 0.78 to 0.83. Additionally, we confirmed 20 influential features through feature importance analysis.

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Poster Presentation : **MAT.P-320**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Broadband-Spectrum Solar Energy Utilization with Lanthanide-doped NaYF4–Au–TiO2 Ternary Hybrid Nanostructures

Sunghee Kang, Sang Woo Han[1,*]

Korea Advanced Institute of Science and Technology, Korea

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

Harvesting full-spectrum solar energy is a critical issue for developing high-performance photocatalysts. Here, we report a hierarchical heteronanostructure consisting of upconverting, plasmonic, and semiconducting materials as a solar-to-chemical energy conversion platform that can exploit a wide range of sunlight (from UV to near-infrared). Lanthanide-doped $NaYF_4$ nanorod–spherical Au nanocrystals–TiO_2 ternary hybrid nanostructures with a well-controlled configuration and intimate contact between the constituent materials could be synthesized by a wet-chemical method. Notably, the prepared ternary hybrids exhibited high photocatalytic activity for H_2 evolution reaction under simulated solar and near-infrared light irradiation due to their broadband photoresponsivity and strong optical interaction between the constituents. Through systematic studies on the mechanism of energy transfer during the photocatalysis of the ternary hybrids, we revealed that upconverted photon energy from the upconversion domain transfers to the Au and TiO_2 domains primarily through the Förster resonance energy transfer process, resulting in the enhanced photocatalysis.

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Poster Presentation : **MAT.P-321**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Low-Temperature Layer-by-Layer Growth of Semiconducting Few-Layer γ-Graphyne to Exploit Robust Biocompatibility

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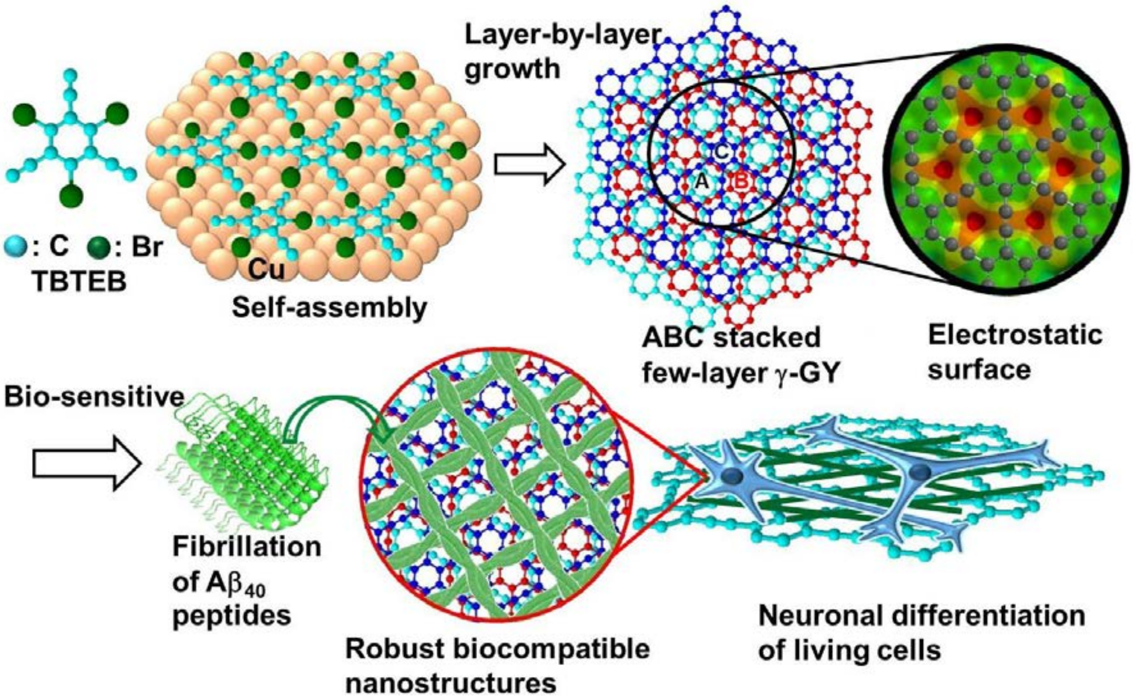
[1] *CINAP-IBS, Department of Chemistry, Sungkyunkwan University, Korea*

The sp-hybridized carbon network in single- or few-layer γ-graphyne (γ-GY) has a polarized electron distribution, which can be crucial in overcoming biosafety issues. Here, we report the low-temperature synthesis, electronic properties, and amyloid fibril nanostructures of electrostatic few-layer γ-GY. ABC stacked γ-GY is synthesized by layer-by-layer growth on a catalytic copper surface, exhibiting intrinsic p-type semiconducting properties in few-layer γ-GY. Thickness-dependent electronic properties of γ-GY elucidate interlayer interactions by electron doping between electrostatic layers and layer stacking-involved modulation of the band gap. Electrostatic few-layer γ-GY induces high electronic sensitivity and intense interaction with amyloid beta (i.e., $A\beta_{40}$) peptides assembling into elongated mature $A\beta_{40}$ fibrils. Two-dimensional biocompatible nanostructures of $A\beta_{40}$ fibrils/few-layer γ-GY enable excellent cell viability and high neuronal differentiation of living cells without external stimulation.


: C
: Br
TBTEB
Cu
Self-assembly
Layer-by-layer growth
A
B
C
ABC stacked few-layer γ-GY
Electrostatic surface
Bio-sensitive
Fibrillation of Aβ40 peptides
Robust biocompatible nanostructures
Neuronal differentiation of living cells

Poster Presentation : **MAT.P-322**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Plasmon-Driven Nanoreactors: Tailoring Catalysis at the Nanoscale

Anubhab Acharya, Seunghyeon Jie, In Su Lee[1,*]

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

Plasmonically coupled nanoreactors, sought after for their ability to efficiently harness light energy for catalytic transformations, are experiencing a significant demand in the catalysis field. The advancement of innovative synthesis techniques is pivotal for engineering intricate nanoarchitectures with multiple functionalities, thereby enhancing their overall efficacy. Our focus lies in achieving this through the precise modulation of nanostructural features and the integration of various components with plasmonic nanocrystals within a nano-confined environment, referred to as a nanoreactor. This discussion aims to showcase our accomplishments in designing plasmonically integrated nanoreactors, emphasizing (i) the implementation of unique synthesis strategies for creating hybrid plasmonic-catalytic interface, (ii) the exploration of plasmonic photochemical reactions, and (iii) the detailed elucidation of the mechanistic pathways involved in these processes. Overall, the presentation will explore the principles behind designing diverse plasmonically coupled nanoreactors, highlighting their capacity to achieve superior performance by effectively utilizing plasmon-induced energy in catalytic transformations.

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Poster Presentation : **MAT.P-323**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Density functional study on the competitive oxidation of water and chloride in seawater electrooxidation by MnO2-deposited Ta-RuO2

Youngha Kweon, Minho Kim[1,*]

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The water splitting reaction is a well-known strategy for energy conversion utilizing water. Despite directly use seawater for this purpose, its high concentration of chloride ions (e.g., NaCl) promotes the chloride oxidation reaction prior to water oxidation, resulting in the generation of Cl2 or HClO. Therefore, it is urgent to selectively promote the oxygen evolution reaction (OER) that competes with the chloride oxidation reaction in seawater. RuO2 is known as a catalyst with low overpotential for the OER, and its activity and stability are often enhanced by a high-valent metal dopant such as Ta5+. However, in the case of Ta-RuO2, both the OER and chlorine evolution reaction (CER) occur competitively. In this study, we purpose to suppress chloride oxidation reaction by an interfacial interaction between catalytic Ta-RuO2 and a MnO2 nanocluster. Based on density functional theory (DFT) simulation, defective antifluorite MnO2 (DA-MnO2) clusters on Ta-RuO2 enhance the *O adsorption and prevent the Cl-O bond association, unlike γ-MnO2 clusters. Furthermore, the Ta-RuO2 with DA-MnO2 clusters is less sensitive and hardly deactivated by chloride adsorption, indicating that the deposition of a proper MnO2 cluster on Ta-RuO2 can lead a selective and preferable oxidation of water to chloride in seawater electrooxidation.

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Poster Presentation : **MAT.P-324**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Photoinduced redox-switchable σ-holes: further application to photovoltachromic cells

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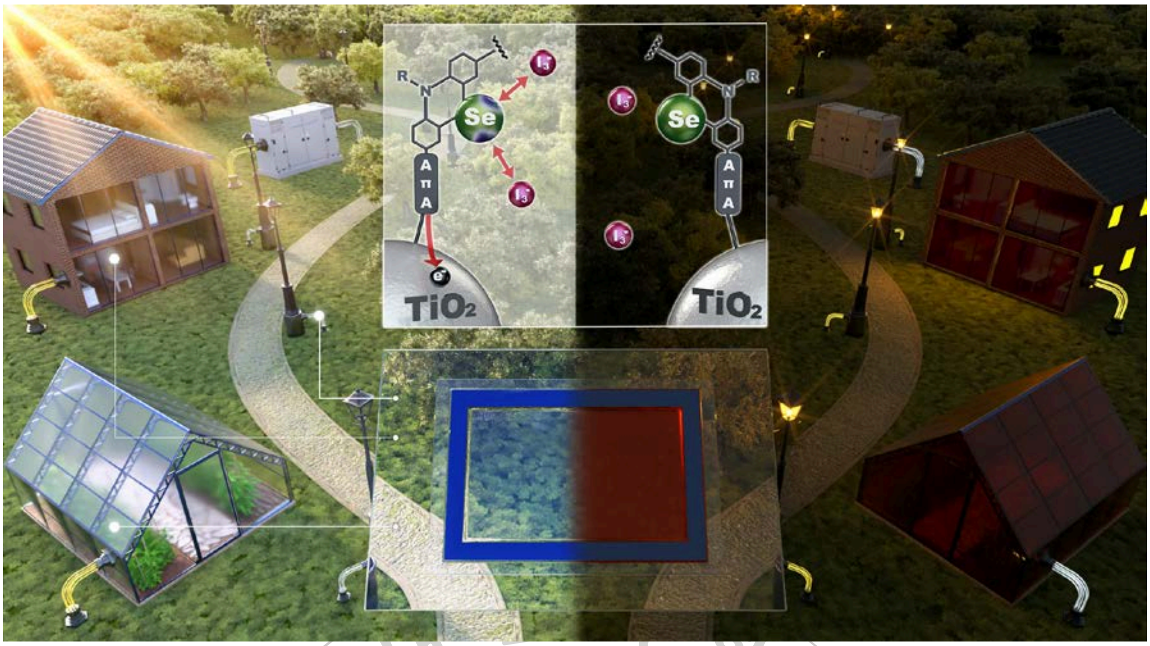
Chalcogen bonding (ChB) is emerging as a powerful noncovalent interaction that can be exploited invarious fields. Here, we first report photoredox-switchable ChB using chalcogen-bonding dye (ChB-dye)that can modulate ChB strength by light and selectively interact with I−/I3− anions. We elucidated themechanism of photoredox-switchable ChB by various spectroscopic and electrochemical techniques. Inaddition, we applied the selenium-based ChB-dye as a dye for photovoltachromic cells (PVCCs), which canfunction as both a solar cell and a smart window without an additional electrochromic layer. PVCC showsa remarkable reversible color change resulting 48% average visible transmittance (AVT) change.


R
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Poster Presentation : **MAT.P-325**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

A ubiquitous polymerization method for modifying the surface properties of inorganic nanoparticles

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Quantum dots (QDs) with stable and narrow photoluminescence (PL) characteristics have emerged as a promising option for diverse biomedical and photovoltaic applications. These QDs exhibit colloidal stability and facile surface modification in a biological medium. The predominant synthetic methods for QDs have been established in organic solvents using oleic acid and oleylamine as surface passivating ligands. To enable their use in various applications, the original hydrophobic surface ligands have been exchanged with additional ligands. A new approach has been developed for dispersing QDs in the aqueous phase without removing the original ligands. This approach preserves the original physical and optical stability of the QDs in water. This method avoids reduced PL stability and etching of the outmost inorganic surface of QDs. The approach involves two reaction steps: epoxidation and nucleophilic addition of hydrophilic ligands or macrocyclic molecules onto the original hydrophobic ligands. This method utilizes post-modification to perform in situ polymerization reactions on the surface of QDs, enabling their incorporation into various types of polymers. This approach offers advantages for the development of sensors or drug-releasing nanoplatforms containing QDs and other nanoparticles.

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Poster Presentation : **MAT.P-326**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Development of colorimetric sensing platform of viral infection using trans-cleavage

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Following the COVID-19 pandemic, the prompt detection of viral infections in the human body has become a crucial issue. The conventional methods of PCR or fluorescence-based sensing have limitations, such as time consumption and the need for experts and equipment, resulting in a failure to achieve early diagnosis and quarantine. A strategy was developed for Point-of-Care Testing (POCT) that utilizes the properties of gold nanoparticles and the CRISPR/Cas system to provide rapid visual confirmation of the presence of a target sequence, such as viral genetic material. This allows for direct observation with the naked eye. When the CRISPR/Cas system recognizes and cleaves the specific target sequence, a trans-cleavage of surrounding ssDNA occurs. A colorimetric sensing platform can provide a true/false indication on site, depending on the amount of leftover ssDNA. This method can be used for diagnostics to rapidly confirm the presence of target genetic material in various biological samples. It can also be used in convenient and useful diagnostic kits for the general population.

Poster Presentation : **MAT.P-327**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Multidentate surface ligands for excellent long-term colloidal stability of QDs

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Bioimaging probes and signal reporters for ultrasensitive in vivo and in vitro applications require exceptionally stable probes that can withstand physiological conditions for extended periods. To address this need, we designed a new multidentate ligand composed of three dithiol groups per ligand as anchoring moieties to the surface of quantum dots (QDs). This design ensures a much higher binding affinity to the QD than conventional monodentate ligands due to the low chance of detaching all the anchoring moieties at once. The colloidal stability of QDs can be significantly improved in physiological media, including broad pH and salt conditions, cell culture media, reducing environments, and storage in buffers with low QD concentrations or plasma. This enhanced stability allows for use after various shipping and storage conditions and systemic delivery into small mouse models.

Poster Presentation : **MAT.P-328**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Theoretical study on the significance of a reducing agent for the preparation of NiSe nanosheet as a hydrogen evolution reaction catalyst

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The hydrogen evolution reaction (HER) is an important reaction for the imperative shift towards sustainable energy conversion and storage. Hydrogen is a clean energy source and stands out among various energy sources for its renewable property. This study focuses on hydrogen evolution reaction in a nickel selenide catalyst model based on the density functional theory (DFT) calculation. The boron-doped NiSe (B-NiSe) nanosheet that was constructed by the commonly used boron-based reductant results in high overpotential for HER, indicating that the utilization of the boron-based reductant can undermine the HER activity of the NiSe catalysts. On the other hand, the NiSe that was constructed by a non-boron reductant and thus does not contain boron dopants (H-NiSe) showed lower overpotential for HER. The projected density of state (PDOS) suggests that the B 2p states in B-NiSe appear to hybridize with Se 4p states. The B 2p states form a strong π bond with Se 4p states that disturbs the formation of Se-H bonds for an HER intermediate in B-NiSe. Therefore, the thermodynamic preference of H binding is weakened and the HER activity of B-NiSe decreases. As a result, our theoretical understanding can suggest the significance of the utilization of non-boron reductant for the preparation of NiSe-based HER catalysts.

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Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Theoretical study on the mechanism of glycerol oxidation reaction on high entropy alloy

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With a rise of the need for eco-friendly energy, the production of glycerol has increased as a by-product of ether in biomass conversion. Therefore, research on glycerol oxidation reaction (GOR) by electrocatalysts to make the overproduced glycerol into a valuable substance has recently attracted attention. As GOR progresses, various kinds of valuable acids, including the most oxidized formic acid, can be produced. Since he catalysts mainly used in this reaction are precious metals such as Au, Pt, and Pd, Non-precious metals must be used to reduce costs. Mo, which shows high activity among these catalysts, has the disadvantage of being easily corrosion. DFT simulation was performed by constructing several high-entropy alloys (HEAs) with Ni, Fe, Co, Mn, and Mo, which are substantially present on the Earth. The activity in the absence of each element was also compared for the optimal composition of alloy catalysts. As a result, the HEA with the highest activity was suggested by descriptors based on the mechanistic understanding of this work. Not only the optimization of GOR electrocatalysts, but it is also expected that the theoretical understanding on GOR in this work will provide electronic and geometric descriptors for the a *priori* design of GOR electrocatalysts.

Poster Presentation : **MAT.P-330**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Synthetic Design of M^{n+}-Condensed DNA Nanoparticles for Nucleic Acid Therapeutics Using Library Approach.

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Department of Materials Science and Engineering, Korea University, Korea

Metal ion (M^{n+})-condensed DNA nanoparticles (CDNPs) are of great interest in the field of nanotechnology and nucleic acid chemistry owing to their distinctive material properties and gene delivery efficacy compared to those of the traditional synthetic DNA nanostructures. To date, however, only a few M^{n+}s including Fe^{2+}, Cu^{2+}, Ln^{3+} and Au^{3+} have been reported as the precursors for the CDNP synthesis. And yet a systematic investigation of the M^{n+}-dependent properties of the CDNPs is in great demand. In this presentation, we synthesized the CDNPs using a library of 30 different M^{n+}s and analyzed the M^{n+}-dependent synthetic routes and gene delivery efficacy of the CDNPs. Gold nanoparticles (AuNPs) are employed as an electron microscopic tracker of the dynamic phase mobility of the CDNPs owing to their advantageous properties such as intense localized surface plasmon resonance and a large atomic number of Au, ideal for optical and electron microscopic analysis. Furthermore, the relative gene delivery efficacies of each CDNP as a function of the M^{n+}s are thoroughly investigated using cancer-treating therapeutic oligonucleotides.

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Material Chemistry

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Electrochemical driven synthesis of Ultrathin 2D-Cu metal atomic layer deposition for Catalysis

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

Developing cost-effective alternatives like copper (Cu) based catalysts for commonly used precious and rare noble metals is crucial for industrial-scale sustainable fine-chemical synthesis. However, controlling and understanding the intricate surface chemistry of Cu at the nanoscale is highly challenging due to its kinetic instability, susceptibility to oxidation, and restructuring that leads to structural disproportionation during catalysis. Designing model catalyst platforms, especially by synthesizing ultrathin 2D-Cu layer sandwiched inside a bilayer silica template, anomalously enables deciphering the critical cooperative role of Lewis basic amino-silica microenvironment for [Cu]-catalyzed selective hydrogenation of unsaturated C—C bonds in diverse alkynes, ene-ynes, and α,β-unsaturated (alkene) Michael acceptors. By utilizing the nanospace-confined electrochemical (eChem) atomic layer deposition (NC-EAD) technique, ultrathin growth of Cu(0)-layer within (< 2 nm thickness) the silica envelope was synthesized. This model platform paved the way for deciphering detailed mechanistic insights on the concept of reactive metal surface-microenvironment, establishing a new paradigm for controlling complex molecular interactions in heterogeneous catalysts.

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Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Non-ammonia nitridation agents for the synthesis of transition metal nitrides and oxynitrides

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

Transition metal (oxy)nitrides garnered much attention recently due to the diverse functionalities suitable for photocatalysts, pigments, and dielectrics. So far, ammonia has served as a popular and efficient nitriding reactant, but in the long run, it will have to be replaced due to biohazardous issues. In this regard, we explored alternative nitridation agents to ammonia and found that small nitrogen-containing organic molecules such as urea, melamine, guanidine, and creatine are useful for the nitridation reaction. Meanwhile, common ammonium salts in the types of chloride, nitrate, acetate, and sulfate did not exhibit any reactivity toward nitride formation. In this study, perovskite oxynitride $BaTaO_2N$ was prepared from $BaCO_3$ and Ta_2O_5 with various nitridation agents (ammonia, urea, guanidine, creatine), and the results are compared in terms of reaction rate, purity control, and optical property of the product.

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Material Chemistry

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Synthesis and performance evaluation of cobalt-free LiNi0.5Mn0.5O2 as cathode materials for lithium-ion batteries

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As the use of lithium-ion batteries increases, the development of low-cost, high-capacity cathode materials is becoming more important. Recent advancements in layered Li(Ni1-x-yMnxCoy)O2 (NMC) cathodes have focused on optimizing energy performance and cost-effectiveness by increasing nickel content while minimizing cobalt content. More importantly, concerns persist regarding the elevated cost and environmental impact associated with cobalt. Co-free LiNi0.5Mn0.5O2 (LNMO) has recently emerged as a promising alternative cathode material capable of meeting these criteria. This study focuses on synthesizing LNMO with a layered structure through a solid-state reaction method using hydrothermally synthesized β-MnO2 nanorods. The LNMO cathodes were tried to synthesize at different temperatures ranging from 700°C to 1000°C. Their physico-chemical properties were systematically characterized. The electrochemical analysis revealed that the LNMO prepared at 900°C exhibited the highest discharge capacity (ca. 222mAh/g) within the operational voltage range of 2.5~4.6V. This finding underscores the potential of LNMO to achieve superior energy density, positioning it as a significant contender in the advancement of battery technology.

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Poster Presentation : **MAT.P-334**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancing Solid Oxide Fuel Cell Performance through Thin Electrolyte Electrolyte-Supported Cells

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Solid oxide fuel cells (SOFCs) represent an innovative approach to power generation, efficiently converting chemical energy into electricity and heat through electrochemical reactions while minimizing pollutant emissions. Among different SOFC cell structures, electrolyte-supported cells (ESCs) have garnered attention due to their dense electrolyte membrane and thin anode and cathode electrodes. These facilitate enhanced sealing at the cell periphery. Despite these advantages, ESC-based SOFCs face challenges in ion conductivity attributed to thicker electrolytes (150-250 μm) compared to Anode-Supported Cells ASCs (Anode-Supported Cells, 10 μm thickness). Achieving a balance between ion conductivity and mechanical strength is crucial. In this work, we used a thin 3-YSZ electrolyte (3mol% yttria-stabilized zirconia) with a thickness of 30~40μm to address this challenge and optimize performance. Fuel electrodes was composed of Ni/YSZ composites, while the air electrodes consisted of GDC/LSCF (La0.6Sr0.4Co0.2Fe0.8O3-δ) composites. SOFC performance was optimized by adjusting the composition of nickel and YSZ in the fuel electrode. The optimized ESC cell achieved a current density of up to 0.32A/cm2 (at 0.7 V and 780℃) cell with excellent stability.

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Material Chemistry
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Enhanced Synthesis of Hematite Photoanodes via Photosintering for Efficient Photoelectrochemical Water Splitting

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Hematite (Fe_2O_3) is a promising candidate for photoelectrochemical (PEC) water splitting due to its narrow band gap (~2.1 eV, corresponding to solar to hydrogen conversion efficiency (STH) 12.9%) and excellent structural and chemical stability under alkaline conditions (> pH 13). In the synthesis of hematite photoelectrode, typically, conventional synthesis methods using electric furnaces face challenges in terms of reliability and time efficiency, often requiring two-step heat treatments. In this study, we employed a photosintering method utilizing a laser diode (ex., vertical cavitiy surface emitting laser, VCSEL) address these issues. This facilitates the rapid synthesis of hematite photoanodes at 780℃ within minutes, as confirmed by X-ray diffraction (XRD) analysis. Under PEC performance condition (1sun, 1M KOH, pH 13.6), the photocurrent density of the photosintered films was approximately exhibited twice as high as that obtained from the conventional electric furnace method reported by previous reports[1]. Moreover, the present photosintering method enables facile doping with various elements such as Zr, Pt, and Ti in a tetravalent oxidation state, thereby offering enhanced versatility and ease of processing.[1] J. Phys. Chem. B, 2005, 109, 13685-13692Key word: Photoelectrochemical water splitting, Rapid sintering, Photoanode, Hematite

Poster Presentation : **MAT.P-336**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Two Distinct Formation Pathways of 2D Wurtzite-CdSe Quantum Nanocrystals Revealed by In Situ X-ray Scattering

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Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Understanding the formation mechanism of quantum-sized semiconductor nanocrystals is key to controlling their synthesis for diverse uses. Previous studies on the formation process of 2D CdSe nanocrystals primarily used ex-situ analyses, leaving gaps in understanding their formation stages and lateral shape evolution. This study explores the growth pathways of two distinct wurtzite-CdSe nanocrystals (i.e., nanoribbons, and nanosheets) using both in situ small-angle X-ray scattering and other ex situ analytical methods. Although both types of CdSe nanocrystals have a similar thickness of approximately 1.4 nm, their lateral sizes are significantly different. We uncovered that the reactivity of the Se precursor is important in determining their distinct growth pathways. High reactivity of precursors leads to nanocluster-lamellar structures, resulting in the formation of elongated 2D nanoribbons. On the contrary, less reactive precursors lead to nanosheets formation from small 2D seeds, with their lateral growth by the effect of chloride ions, instead of nanocluster-lamellar structures or Cd(halide)2–alkylamine frameworks, leading to shorter 2D nanocrystals. This work provides insight into a growth mechanism of quantum-sized 2D semiconductor nanocrystals, offering important guidelines for their systematic synthesis.

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Poster Presentation : **MAT.P-337**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Ce-MOFs derived Ce-Mn bi-metal oxide catalysts for CO oxidation

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CeO_2-based catalysts are widely studied in the catalysis fields. Developing one novel synthetic approach to increase the intimate contact between CeO_2 and secondary species is of particular importance for enhancing catalytic activities. Herein, we design an interfacial reaction between MOF-derived Carbon and $KMnO_4$ to synthesize CeO_2-MnO_2, where the Carbon is derived from the pyrolysis of Ce-MOFs under inert atmosphere. The MOF-derived Carbon is found to restrain the growth of CeO_2 crystallites at high calcination temperature, and more importantly, the intimate contact within CeO_2/C is conveyed to CeO_2/MnO_2 after interfacial reaction, which are responsible for high catalytic activity of CeO_2-MnO_2 towards CO oxidation.

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Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Non-invasive Cystine Monitoring Contact Lenses with the Color Change in Gold Nanoparticles

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Ocular cystinosis is a disease caused by the accumulation of cystine crystals in the eyes, leading to symptoms such as photophobia and even blindness. This disease needs timely monitoring of cystine accumulation, but current diagnostic methods have limitations because of invasive blood sampling. Herein, we aimed to develop gold nanoparticle contact lenses (GNP-CL) utilizing its strong affinity with cystine sulfur, for non-invasive monitoring of cystine levels. We synthesized monodisperse gold nanoparticles (GNP) of 15nm. Our initial focus was on verifying the interaction between GNP and cystine in an aqueous solution. The confirmation of binding was established through the amorphous interface encapsulating GNP in TEM images. As cystine concentrations increased, GNP reacted with cystine to induce more aggregation. Due to the inherent characteristics of GNP, the original red color shifted to blue. Subsequently, we developed GNP-CL by loading the contact lens into the GNP solution. According to the cystine concentration, the hue value of the lens changed, and the cystine concentration (40uM) showed a change of about 30%. The Hue value according to the cystine concentration showed a linear section up to about 30uM, and based on this, it is confirmed that it is possible to monitor the cystine concentration in tears.In this study, the reactivity of GNP and cystine was confirmed both in the aqueous solution state and contact lens. The gradually changing color of the contact lens according to the cystine concentration shows the possibility of non-invasively confirming the cystine level instead of the currently used invasive monitoring. The reaction between GNP-CL and cystine could potentially aid in the therapeutic process by removing cystine from the tear fluid.

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Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Magnetic field-directed monolayer assembly of plasmonic nanoparticles

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Two-dimensional (2D) monolayer films of nanoparticles have attracted tremendous interest due to their distinctive optical, and electrical characteristics. In this study, magnetoplasmonic ($Ag@Fe_3O_4$) nanoparticles were self-assembled at the interface of two immiscible liquids to form a densely packed 2D monolayer film. This 2D nanoparticle array is partially embedded into the polymer surface, remaining readily accessible for physiochemical interactions. The resulting two-dimensional arrays enable tunable colors based on the sizes of the nanoparticles. Due to the distinct magnetic property of iron oxide shell, $Ag@Fe_3O_4$ nanoparticles can be directionally assembled upon exposure to a magnetic field. These magnetic field-responsive plasmonic nanoparticles offer a promising premise for imaging and chiroptical applications.

Poster Presentation : **MAT.P-340**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Investigation into Enhanced Conductivity of Na6ZnSe4-based Sodium Solid-State Electrolyte (Na-SSE) via Elemental Dopant Integration

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The rising demand for high-performing, safe, cost-efficient, and environmentally sustainable batteries have underscored the importance of developing electrolytes with superior characteristics such as enhanced performance, lower volatility, and thermal stability. This study explores the potential of Na6ZnSe4 as a sodium-solid-state electrolyte (Na-SSE), examining its hexagonal structure for efficient sodium conduction. Despite achieving phase-pure Na6ZnSe4 through various synthesis methods, the obtained conductivity remains relatively low (~0.05 µS/cm). Current efforts are directed towards enhancing conductivity by fine-tuning the crystallographic structure through dopant integration. This involves varying dopant concentrations to optimize the material's properties. The ultimate goal of this research is to contribute to the advancement of electrolyte technology for the development of next-generation battery systems.

Poster Presentation : **MAT.P-341**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Optimizing Alkyl Chains of Non-fullerene Acceptors for Enhanced Printability in Organic Photovoltaic Modules Over 200 cm^2 Using Non-halogenated Solvent

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Organic solar cells (OSCs) offer sustainable energy solutions with advantages like light-weight and flexibility. The solution-processibility of organic materials enables the economical fabrication of large-area organic solar modules. However, the prevalent use of toxic halogenated solvents (e.g., chloroform, chlorobenzene, etc.) for OSC fabrication raises environmental and health concerns, highlighting the need for alternatives with low toxicity such as non-halogenated solvents (e.g., o-xylene, etc.). Moreover, a critical issue reducing the performance of OSC is the significant aggregation of non-fullerene acceptors (NFAs) causing the unfavorable film morphology during the solidification of the active layer. These problems are worse when fabricating large-area modules which take longer time to solidify active layers. In this work, we developed the NFAs as a derivative of L8-BO(EH-EH) by substituting the original alkyl chains with longer ones on pyrrole to reduce the aggregation of NFAs by increasing solubility of NFAs in o-xylene. Specifically, we replaced the 2-ethylhexyl groups on L8-BO(EH-EH) with longer ones to produce derivatives such as L8-BO(HU-HU), L8-BO(HU-DT), and L8-BO(HU-DH), which show improved solubility and film uniformity in o-xylene. These modifications lead to o-xylene-processed organic solar modules with an area of 200 cm^2 exhibiting power conversion efficiencies over 10%. Comprehensive analyses, including GIWAXS and AFM, demonstrate the effects of alkyl chain optimization on NFA aggregation and film morphology. This work emphasizes the importance precisely optimizing alkyl chains of NFA to enhance film printability and suppress severe aggregation of NFAs in the fabrication of large-area organic solar modules using non-halogenated solvents.

Poster Presentation : **MAT.P-342**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Vacancy-Controlled Quaternary Sulfide $Na_{6-x}Zn_{1-x}M_xS_4$ (614) for All-Solid-State Sodium-Ion Batteries

Seolyeon Kang, Myoungho Pyo[1,*]

Advanced Components and Materials Engineering, Suncheon National University, Korea
[1]*Department of Energy Engineering, Korea Institute of Energy Technology, Korea*

In the area of contemporary commercial secondary batteries, the prevalent use of liquid electrolytes introduces a notable fire hazard during battery operation, attributed to chemical reactions and exothermic processes. Recognizing the imperative need for enhanced safety measures, researchers are delving into innovative strategies, with a particular focus on substituting solid electrolytes for their liquid counterparts in secondary battery designs. While solid electrolytes are commonly associated with lithium-ion batteries, the scarcity of lithium resources presents a fresh set of challenges for researchers. This research endeavors to address these challenges by investigating solid electrolytes, utilizing sodium as a viable substitute for lithium. In this work, the primary objective is to enhance ion conductivity by introducing vacancies through doping in the original Na_6ZnS_4. Specifically, the synthesis of $Na_{6-x}Zn_{1-x}M_xS_4$ compounds involves the substitution of M^{3+} for Zn^{2+} ions. The resulting compounds underwent rigorous examination through X-ray diffraction to validate the absence of impurities. Ion conductivity was systematically evaluated using Electrochemical Impedance Spectroscopy. The findings illuminate a notable increase in ion conductivity with higher doping concentrations, reaching a maximum of 30 μS/cm at x=0.4. This signifies a remarkable advancement, showcasing a four-order magnitude improvement compared to the pristine state's ion conductivity of 0.002 μS/cm. Further in-depth analysis and ongoing electrochemical studies are being conducted.

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Material Chemistry
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Ionic conductivity of Li_3AlSiO_5-based solid solutions derived by Si/P and Si/V substitutions

Song Hyeon Kim, Young-il Kim*

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The compositional control of Li_3AlSiO_5 was made by Si^{4+}/P^{5+} and Si^{4+}/V^{5+} substitutions, where the lattice volume, covalency, and cation order were modified. In both cases of P and V, substitution could be achieved up to 5 mol%. Among $Li_{2.95}Al_{0.95}Si_{1.05}O_5$, $Li_{2.95}AlSi_{0.95}P_{0.05}O_5$, and $Li_{2.95}AlSi_{0.95}V_{0.05}O_5$, the lattice volume varied in consistency with the ionic radii of Al^{3+} (0.39 Å), Si^{4+} (0.26 Å), P^{5+} (0.17 Å), and V^{5+} (0.355 Å), and it is presumed that the pentavalent substituents gave rise to increased lattice covalency. As measured by the ac impedance spectroscopy, the ionic conductivity was $2.41 \times 10^{-5} \Omega^{-1} cm^{-1}$ at 500 °C

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Poster Presentation : **MAT.P-344**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancing Performance through Effective Passivation Strategies in InAs Quantum dots

Sinil Choi, Sohee Jeong[*]

Department of Energy Science, Sungkyunkwan University, Korea

The field of quantum dots has gained considerable attention owing to their unique optical and electronic properties, and InAs-based quantum dots, in particular, have emerged as a spotlighted candidate for various applications. The success of these applications, however, hinges on effective passivation strategies to enhance stability and performance. This work delves into the intriguing realm of passivation techniques and the burgeoning applications of Near-Infrared to Short-Wave Infrared (NIR-SWIR) quantum dots, specifically focusing on InAs. We have successfully completed the Zn, ZnSe shelling process, achieving a photoluminescence quantum yield (PLQY) greater than 75%, full-width half maximum (FWHM) of 140 meV, and a peak photoluminescence wavelength (PLmax) at 950 nm. We anticipate that the findings from this study can be applied to various applications in the future.

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Poster Presentation : **MAT.P-345**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Extended-Gate Field-Effect Transistor (EGFET) Biosensor with Nanoscale Surface Roughness of Sensing Membrane for Ultra-Sensitive Detection of Alzheimer's Disease Biomarker

Hana Kim, Young-Geun Ha[*]

Department of Chemistry, Kyonggi University, Korea

Biosensor-based field-effect transistors are ideal for point-of-care diagnostics, but their sensitivity declines due to electrical double layers (EDLs) that partially screen potential changes. To address this issue, we utilized the nano-scale roughness of the sensing membrane surface, which serves as a sensing membrane. We adopted a cost-effective, rapid, and highly selective wet etching process, leveraging simple equipment to fabricate these surfaces. The nano-scale roughness increased the number of binding sites and reduced Debye screening, consequently amplifying the sensitivity of the EGFET biosensor. Moreover, our investigation found that the nanoscale surface roughness of the sensing membrane was associated with a further increase in sensitivity. To achieve stable results, we opted for an extended gate field-effect transistor (EGFET) structure. The EGFET structure also allows for the omission of the passivation process, simplifying the fabrication process and reducing costs. Our approach is fast, simple, stable, and cost-effective, rendering it a promising strategy for enhancing the performance of various EGFET biosensors and improving the utility of point-of-care diagnostic devices in practical settings.

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Poster Presentation : **MAT.P-346**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Improving Sensitivity of Electrolyte-Gate Field-Effect Transistor-Based Biosensors by Controlling Conductance of Semiconductor

Euichan Jeon, Young-Geun Ha[*]

Department of Chemistry, Kyonggi University, Korea

Field effect transistors (FETs) are being used in various ways in the field of biosensors. In this study, various performance biosensors were fabricated using an electrolyte-gate field effect transistor based on IGZO semiconductors. To compare the performance of biosensors according to semiconductor conductivity, devices with different conductivity were manufactured to compare sensitivity. All types of manufactured biosensors have successfully detected tau protein, a target substance for Alzheimer's disease. The electrode passivation method used SAML (self-assemble multilayer) with excellent insulation for operation safety. In addition, the sol-gel process of the semiconductor film and the surface treatment of the sensing region are performed through a solution process, which has the advantage of fabricating the sensor in a simple and low-cost method.

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Poster Presentation : **MAT.P-347**
Material Chemistry
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Nanoimprinted Semiconductor Surfaces for Improving the Sensitivity of Electrolyte-Gated Field-Effect Transistor Biosensors

Gyeongmin Lee, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

Biosensors are vital devices used to detect and quantify biological analytes in samples, with electrolyte-gated field-effect transistors (EGFETs) particularly suited for point-of-care diagnostics (POCD). However, electrolytes in this system lead to the formation of electrical double layers (EDLs) on the semiconductor surface, causing debye screening that interferes with surface potential changes, significantly reducing sensor sensitivity. To address this, nanoimprint lithography was used to create nanoscale patterns on the semiconductor surface. Patterns from optical discs were transferred onto the semiconductor surface using poly(dimethylsiloxane) (PDMS) as a template. These nanoscale patterns effectively suppress EDL formation in concave structures, reducing debye screening and enhancing sensor sensitivity.

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Poster Presentation : **MAT.P-348**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Self-Assembled Multilayer-Based Electrode Passivation for Stable and Reproducible Electrolyte-Gated IGO Transistor Biosensors

Hye-Seon Kim, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

To maintain the operational stability of transistor-based biosensors in aqueous electrolytes, effective electrode passivation is crucial. We propose a highly efficient passivation method using a solution-processed self-assembled multilayer (SAML) for electrolyte-gated transistor (EGT) biosensors. The SAML structure, composed of layers of 1,10-decanedithiol, vinyl-polyhedral oligomeric silsesquioxane, and 1-octadecanethiol, ensures the reliable functioning of EGTs in phosphate-buffered saline (PBS) without short-circuiting over multiple cycles. The SAML-passivated EGT biosensor is fabricated with a solution-processed IGO thin film as an amorphous oxide semiconductor working both as a semiconducting channel in the transistor and as a functionalizable biological interface for a bioreceptor. This highlights the effectiveness of the SAML passivation technique in achieving stable and reproducible biosensors.

Poster Presentation : **MAT.P-349**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Study on Creating Robust and Superior Superhydrophobic Surfaces Using an Economical and Simple Solution Process at Room Temperature

Ju-Hyeok Lee, **Young-Geun Ha***

Department of Chemistry, Kyonggi University, Korea

The superhydrophobic properties observed in natural elements like lotus leaves, salvinia leaves, and beetle exoskeletons have advanced extensive research in biomimicry. To coat surfaces with these properties inexpensively, we developed a two-step solution-based coating process at room temperature. Initially, a metal precursor solution was sprayed to create a rough metal oxide surface, followed by etching and the formation of a Self-assembled Monolayer (SAM) using Octadecylphosphonic acid (ODPA) solution. This yielded surfaces with a water contact angle (WCA) exceeding 150° and a sliding angle of approximately 10°, demonstrating excellent superhydrophobicity. Our method is applicable to various substrates, including fabrics, silicon, and glass, offering a cost-effective and simple solution with superior superhydrophobic properties for wide practical applications.

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Poster Presentation : **MAT.P-350**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Passivation Layer Formation on Organic Transistor Surfaces utilizing Superhydrophobic Nanoparticles

Ieon Park, Young-Geun Ha*

Department of Chemistry, Kyonggi University, Korea

OFETs are next-gen organic electronic devices, applicable to paper-like, thin, and flexible substrates through cost-effective solution processes. However, a persistent challenge in organic electronics and oxide semiconductors is their long-standing issue of low stability in open environments, particularly poor water resistance.we created a superhydrophobic protective film with substituted nanoparticles, effectively resolving these concerns. The film repels water, possesses self-cleaning properties, and shows excellent resistance to water, NaOH, and HCl exposure, ensuring stable electrical characteristics. Furthermore, it functions efficiently when exposed to PBS solution, indicating potential biosensor applications.These findings significantly enhance organic electronic device stability, fostering various applications and novel technology advancements.

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Poster Presentation : **MAT.P-351**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Density functional study on iridium-based electrocatalyst for an active and stable oxygen evolution reaction in acidic media

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Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Oxygen Evolution Reaction (OER) have attracted interest for renewable conversion of electricity based on an electrochemical water splitting method. While OER under an alkaline condition is highly developed over decades, OER under an acidic media has been questioned for low stability of noble metal oxides (RuO2 and IrO2) despite its advantage of high proton conductivity. In this study, we suggest a design principle of a highly active and stable Ir-based oxide catalyst based on a nanoparticle model on MnO2 surface to maintain efficiency and stability under acidic conditions while reducing costs. We compared three categories of nanostructures – rutile IrO2 as bulk structure, nanocluster IrO2 as a confined but finite-sized nanostructure, and single-atom Ir catalyst on MnO2. Density functional theory (DFT) calculations confirmed that the nanocluster IrO2 on MnO2 shows the lowest overpotential of OER among them, indicating its highest OER activity. Additionally, the nanocluster IrO2 showed the highest dissolution potential of an Ir atom, confirming its stability under working potentials. This work can suggest a promising catalyst to conduct efficient OER with high stability and activity in acidic media based on the size-controlled preparation of IrO2 nanocatalysts with support materials.

Poster Presentation : **MAT.P-352**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Solid Ion Conductor for Li All-Solid-State Batteries based on Y-Cl series structure

Hyeonjin Seo, Inkyoung Han, Haewon Kim, Seung-Tae Hong[*]

Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea

Lithium ion conducting solid electrolytes show promise for enabling high-energy secondary batteries chemistries and solving safety issues associated with conventional lithium batteries. Solid electrolytes may reduce the safety issues associated with liquid-based electrolytes and improve the compatibility with anode and cathode materials over a range of cell voltages. In this work, we synthesized the new composition and structure of solid electrolyte and its currently being analyzed its structure and electrochemical properties. We synthesized those new materials by hand ground and heat treatment methods. In this study, based on the Yttrium chloride structure, we used bond valence sum calculation to find an interstitial site that Li+ could occupy, and attempted to produce a solid Mg2+ ion conductor through the process of inserting Mg into the site using solid-state synthesis. Analysis includes X-ray diffraction and electrochemical impedance spectroscopy. Through structural analysis, we confirmed that a single phase of the basic skeleton structure was synthesized, and we plan to conduct additional research on ionic conductivity.

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Poster Presentation : **MAT.P-353**

Material Chemistry

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Pegylated Oxidized Carbon Nitride nano dots: Free chelator 64-Cu labeling for PET imaging probes.

Taehyun Park, Dong Wook Kim[*]

Department of Chemistry, Inha University, Korea

Radiolabeled nanoparticles are attracting attention as imaging probes to diagnose various diseases in Positron emission tomography (PET)imaging. Previously, chelators had to be used on the surface to label the nanoparticles with radioactive metals. However, functionalized these chelators to nanoparticles was often caused several problems due to absent of functional group in nanoparticle, sensitivity to harsh reaction condition, low functionalization yield. Oxidized carbon nitride (OCN) synthesized carbon nitride (g-C3N4) using the Hummers method. OCN has better water dispersion than conventional g-C3N4, but still has a disadvantage of low water dispersion stability. To solve this problem, Polyethylene glycol (PEG) was combined to increase the water dispersion stability and synthesize a material capable of radioactive metal labeling without a chelator. PEG-OCN has shown high 64-Cu chelator characteristics and ability to target tumors through animal experiments

Poster Presentation : **MAT.P-354**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Growth of Vertically aligned Silicon Nanowires with kinked structure by adjusting parameters

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Silicon nanowires(SiNWs) contribute significantly to advancements in nanotechnology, finding diverse applications due to their unique properties. This paper examines the synthesis methods and key characteristics of Silicon nanowires(SiNWs). Primarily synthesized through chemical, physical, and hybrid techniques, these methods contribute a vital role in controlling the size, shape, and properties of nanowires. Additionally, recent research trends in various application fields of Silicon nanowires(SiNWs), including nanoelectronic devices, solar cells, sensors, and bio applications, are briefly introduced. Finally, discussions encompass the future prospects and research directions of Silicon nanowires(SiNWs).In this study, an advanced CVD method is proposed, capable of controlling the cooling rate post-reaction and residual gases. Introducing new stages post-growth serves as a means to prevent Au migration on the nanowire surface. Lastly, attempts were made to alter the direction of Silicon nanowires(SiNWs) during the growth stage. Through programmed temperature swings, kinked structures of Silicon nanowires(SiNWs) can be achieved even in vertical growth.

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Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Precision Nano Patterning with Oxide Lithography

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chemistry, Hanyang University, Korea
[1]*Department of Chemistry, Hanyang University, Korea*

Oxide lithography has emerged as a promising technique within atomic force microscopy (AFM) lithography for nano patterning due to its versatility and precision. This study explores the application of oxide lithography in fabricating nanostructures with tailored properties and functionalities. The process involves the controlled deposition of an oxide layer on a substrate followed by selective removal through AFM-based lithography. The oxide layer acts as a mask, enabling the creation of intricate patterns on various substrates including semiconductors, metals, and polymers. Moreover, the oxide layer serves as a protective coating, preserving the integrity of the underlying substrate during the patterning process. This not only ensures high fidelity in pattern transfer but also allows for multi-step lithography processes without damaging the substrate. Furthermore, oxide lithography offers excellent control over feature size, shape, and spacing, facilitating the fabrication of complex nanostructures with tailored functionalities. The compatibility of oxide lithography with existing fabrication techniques such as photolithography and electron beam lithography enhances its potential for integration into mainstream nanofabrication processes.In this study, pattern design is achieved utilizing oxide lithography. By adjusting the tip voltage, a metal layer can undergo oxidation within an electrochemical process. This controlled process enables nano-scale patterning to be carried out. Such an approach can find applications across various fields including nanoelectronics, photonics, and biotechnology.

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Poster Presentation : **MAT.P-356**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Innovative Electrospinning Techniques: A Comparative Study of Fiber Alignment Using a Switching System

Soo Jin Roh, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

Electrospinning has emerged as a versatile technique for producing nanofibrous materials with applications ranging from tissue engineering to filtration. This research focuses on an innovative approach to enhance electrospinning by incorporating a switching system to manipulate alignment during the process. The study investigates the impact of the switching system on fiber alignment, aiming to understand and optimize the alignment control in electrospun fibers. The experimental setup involves a unique electrospinning apparatus equipped with a switching system that enables dynamic adjustments during the electrospinning process. Different parameters, such as voltage, pump rate, and switching time, are systematically varied to explore their influence on fiber alignment. The morphology and alignment of electrospun fibers are characterized through SEM and image analysis techniques. This results indicate a significant correlation between the switching system parameters and the resultant fiber alignment. The findings suggest that real-time control over electrospinning conditions allows for the precise manipulation of fiber alignment, offering new possibilities for tailoring material properties. Potential applications of the optimized electrospinning process include the development of biomimetic scaffolds, advanced filtration materials, and controlled-release drug delivery systems.

Poster Presentation : **MAT.P-357**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Growth behaviors and Surface properties of Zincone films grown by Molecular Layer Deposition

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

ABSTRACT:MLD Molecular Layer Deposition is an advanced organic polymer film and organic inorganic hybrid film preparation technology. One molecular layer can be deposited in each cycle. Compared with traditional organic polymer film deposition process, the film thickness can be accurately controlled (controlled cycle number),more uniform thickness, better shape preservation.However, the growth behavior and surface characteristics of the film at the initial stage of growth still need to be studied. In this study, zincone films were prepared by molecular layer deposition on two metal oxide substrates, Al_2O_3 and SiO_2.The growth behavior and surface properties of zincone films were studied experimentally..In addition, the intermolecular interactions in zincone films depend on the thermodynamics of the molecules,leading to binding failures and cross-linking at different growth temperatures. The mas-s change of zincone film was monitored and recorded by insitu quartz crystal microb-alance (QCM), and the molecular geometry and surface binding energy of zincone film on substrate were determined by density functional theory (DFT).

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Poster Presentation : **MAT.P-358**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Selective adsorption of DNA on size-dependent layered double hydroxides

Jing Xie, Jae-Min Oh*

Department of Energy and Materials Engineering, Dongguk University, Korea

Layered double hydroxides (LDHs) with different particle diameters were synthesized, and its adsorption behavior toward deoxyribonucleotide (DNA) was examined with respect to the strand length of DNA. Small-sized LDH (LDH-S) was synthesized by conventional coprecipitation, while large particles (LDH-L) were prepared by urea hydrolysis method. The X-ray diffraction patterns indicated the LDH-L with a higher crystallinity than the LDH-S; LDH-S and LDH-L with average particle sizes of 20 nm and 2500 nm were proved by scanning electron microscopy. Adsorption isotherm revealed that LDH-S had a good agreement with Freundlich model (multilayered-adsorption), while LDH-L followed Sips (a combination of single-layer and multilayer adsorption). The electrophoresis of ladder DNA after adsorption discovered that DNA with less than 800 bp length was more adsorbed by LDH-S than LDH-L; on the contrary, long stranded DNA (>800 bp) was more effectively adsorbed by LDH-L than LDH-S. Picogreen assay showed that the amount of adsorbed DNA increased with LDH/DNA ratio. The large particle size of LDH tended to adsorb a longer length of DNA (>800 bp), and the small particle size of LDH was more inclined to adsorb a shorter length of DNA (

Poster Presentation : **MAT.P-359**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

High-Purity Magnesium Hydroxide synthesis for the Application of Flame Retardants

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Engineering Materials Center, Korea Institute of Ceramic Engineering and Technology, Korea
[1]*Engineering Materials Center, Korea Institute of Ceramic Engineering and Technol, Korea*

Magnesium hydroxide (Mg(OH)2) is used for various applications such as flame retardant because of its has excellent dehydration reaction and heat content at high temperatures. The powders used for flame retardant is important the color, purity, shape. When using dolomite, it is important to remove Fe and Si in dolomite because they affect the color of flame retardant products. Ca and Al ions in the bittern can be removed through various methods such as acid treatment, pH control, and solubility. In this work, we studied the refining/separation process to decrease production cost. Especially, purity/size/shape of Mg(OH)2 can be controlled using NaOH, NH4OH and dolime (heat-treated dolomite) in the precipitation process.The size, shape and physical properties of the synthesized Mg(OH)2 were confirmed using analysis equipment such as Inductively Coupled Plasma (ICP) and X-Ray Fluoresce (XRF).

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Material Chemistry

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Magnesium Hydroxide and Mg fiber Synthesis by Basic/Acid Catalyst

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Magnesium hydroxide and oxide suitable for the use in flame retardants was prepared from bittern by sulfuric acid leaching, precipitation with NaOH, NH4OH. The removal of Ca2+ ions contained in bittern plays an important role in the purity of Magnesium hydroxide. CaSO4 and MgSO4 can be separated through various methods such as acid treatment, pH control, and solubility. In addition, the obtained Mg(OH)2 can obtain 5Mg(OH)2·MgSO4·3H2O whisker(Mg-fiber), a functional material, through pH control through a basic/acid catalyst. We established a process system that can obtain Mg fibers by controlling the ratio of Mg(OH)2, sulfuric acid, and basic catalyst using bittern. The phase and morphology of the as-prepared samples were analyzed by X-ray diffraction(XRD), scanning electron microscopy(SEM) and transmission electron microscopy(TEM).

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Poster Presentation : **MAT.P-361**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Carbon Monoxide-Mediated Synthesis of Atomically Thin Iridium Metallic Nanosheets for Boosting Acidic Oxygen Evolution

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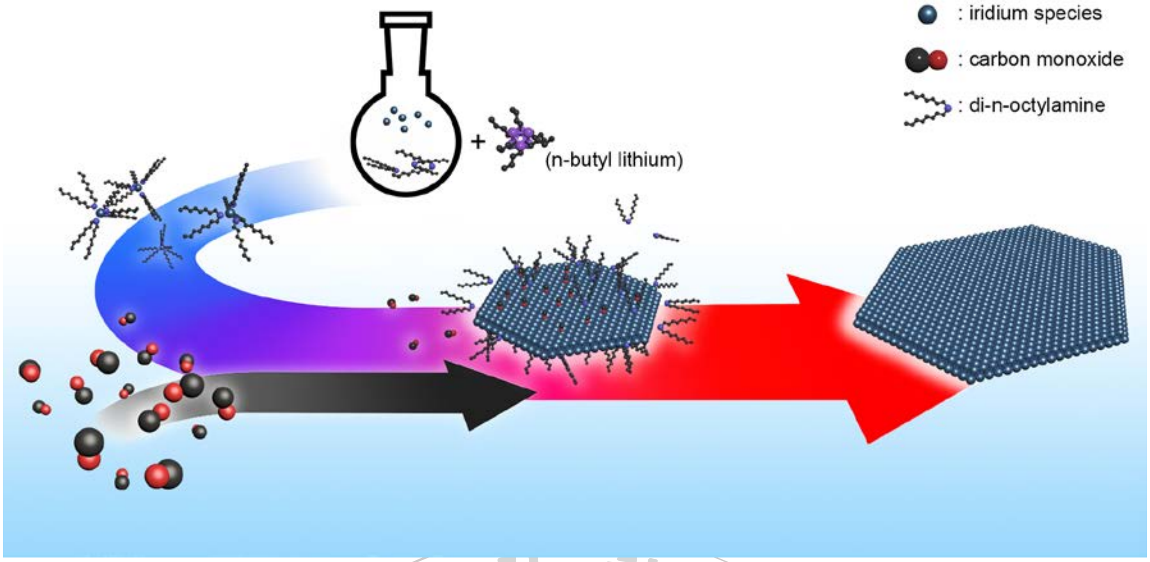
Based on the large surface area, two-dimensional (2D) nanostructures such as nanosheets have many advantages in catalysis. Especially, noble metal-based 2D nanostructures are attractive catalysts because the utilization of the material can be improved a lot. Designing a simple method to synthesize noble metal-based 2D structures can be a big step to making a catalyst with an ultrahigh activity. Here, we report a synthetic method using a carbon monoxide shaping agent to provide ultrathin iridium nanosheets. For the synthesis, iridium and long-chain amine solvent form a complex with the assistance of a strong base. High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) analysis showed that the iridium nanosheets are atomically thin, consisting of only two atomic layers in the thinnest part. Due to the enlarged surface area, the atomically thin iridium nanosheets showed better activity toward the oxygen evolution reaction (OER) in acidic conditions than the commercially available iridium catalysts.


: iridium species
: carbon monoxide
: di-n-octylamine
+
(n-butyl lithium)

Poster Presentation : **MAT.P-362**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

A Study on the Purification of Si3N4 powder using Chemical Method

Yeong Jo Yun, Yoojin Kim[1,*]

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[1]*Engineering Materials Center, Korea Institute of Ceramic Engineering and Technol, Korea*

Silicon nitride (Si3N4) is used for heat dissipation board because it has excellent properties, but it depending on imports. To address these issues, research on development of silicon nitride (Si3N4) manufacturing and processing technology has been vigorously taking place. Therefore, in this study, we studied the purification method using chemical method for synthesis Si3N4 powder. For chemical purification, different acid mixtures based on HCl were prepared, and changes in impurities of metal contents and phase fractions were confirmed. Through acid treatments, the content of Fe ion in the powder could be removed by 90%. The characterization of the purificationed Si3N4 were analyzed using XRD (X-ray diffraction), XRF (X-ray fluorescence), ICP (Inductively Coupled Plasma) and SEM (Scanning Electron Microscope).

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Poster Presentation : **MAT.P-363**

Material Chemistry

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Crystal Growth Characteristics of Magnesium Hydroxide prepared by Hydrothermal Method and Surface Treatment

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Magnesium hydroxide ($Mg(OH)_2$) which is useful for fire-retardants and refractive materials was separated from sea bittern. As a first step, calcium ions were removed as calcium sulfate ($CaSO_4$) by addition of sulfuric acid (H_2SO_4) to sea bittern. By the addition of ammonia (NH_4OH) solution, the pH of bittern solution increased and $Mg(OH)_2$ was precipitated into crystals about several hundred nm in diameter. To induce growth of magnesium hydroxide crystals, hydrothermal methods above boiling temperature of water were proceeded in NH_4OH solutions. Before the hydrothermal method, surface treatments in sodium hydroxide aqueous solution were additionally proceeded and remarkably enhanced the growth of $Mg(OH)_2$ because the surface charges of the $Mg(OH)_2$ crystals played a crucial role to obtain large crystals. The crystal sizes of $Mg(OH)_2$ grew up to micrometer scale and the specific surface area were reduced. The prepared $Mg(OH)_2$ were analyzed by SEM, XRD, TEM, ICP-OES, and TG-DTA.

Poster Presentation : **MAT.P-364**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Solid Ion Conductor for Mg All-Solid-State Batteries based on Y-Cl series structure

Hyeonjin Seo, Seungyong Shin[1], Seongnam Kim[1], Eunchae Song[1], Choi Hosu[1], Seung-Tae Hong[*], Jungmin Park[2]

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[2]*Materials Science and Engineering, Korea University, Korea*

Developing sustainable energy tech is vital. Lithium-ion batteries are widely used but face raw material shortages. Therefore, exploring new chemistry such as magnesium-ion batteries could be an alternative, due to the abundancy and divalent nature. Mg metal also offers higher volumetric capacity (3833Ah/L) as compared to Li metal (2062Ah/L) making it a great anode material candidate.In addition, Mg metal has a significantly higher melting point (650℃) than Lithium metal (180℃) or sodium metal (97.8℃), making it possible to operate at Ultra-High-Temperature. These ultra-high temperature driving batteries can be used in oil drilling, fire suppression, spacecraft, etc. Therefore, we studied solid Mg2+ ion conductor to drive ultra-high temperature Mg all-solid-state batteries. In this study, based on the Yttrium chloride structure, we used bond valence sum calculation to find an interstitial site that Mg2+ could occupy, and attempted to produce a solid Mg2+ ion conductor through the process of inserting Mg into the site using solid-state synthesis. Analysis includes X-ray diffraction and electrochemical impedance spectroscopy. Through structural analysis, we confirmed that a single phase of the basic skeleton structure was synthesized, and we plan to conduct additional research on ionic conductivity.

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Material Chemistry

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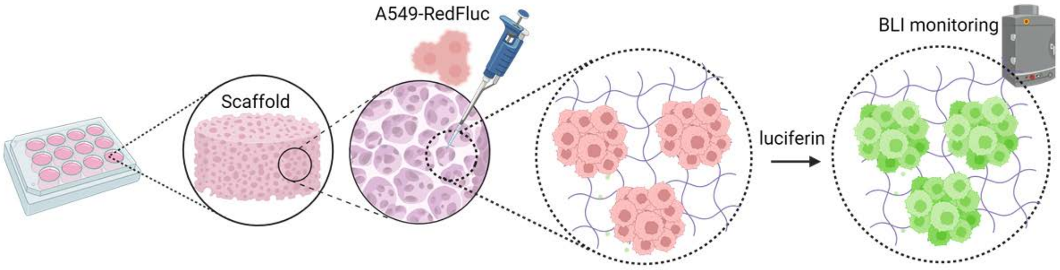
Tumor micro-environment (TME) of A549 lung cancer cells cultured in 3D hyaluronic acid-based scaffold system

Chau Tran

Biopharmaceutical Research Center, KOREA BASIC SCIENCE INSTITUTE, Korea

Immunotherapies using cells have demonstrated impressive clinical results, offering promise for the treatment of cancer. The growing interest in immune cell-based therapies for solid tumors emphasizes the need for long-term observation in experimental models in order to replicate immune cell therapy delivery in clinical settings. This research investigates the potential of cell culture technology based on scaffolds, especially synthesized from hyaluronic acid (HA) which are essential components of the extracellular matrix (ECM) in most body tissues. It provides significant utility in various biomedical application due to its biodegradability, non-immunogenicity, and non-toxic nature. In this study, we developed a meticulous HA-based three-dimensional (3D) cell culture model for A549 lung cancer cells, and investigated the tumor micro-environment and epithelial-mesenchymal transition (EMT) markers depending on time. Compared to conventional 2D monolayer culture system, in our scaffold A549 cancer cells revealed stable growth under spheroid morphology in the scaffold within 30 days. The result showed that the 3D-culture environment upregulated EMT markers, including CD44, vimentin, N-cadherin and fibronectin. Our HA-based scaffold for 3D cell culture model demonstrate a potential tool for reliable applications prior to immunotherapeutic in vivo, providing a suitable basis for research on drug resistance mechanisms and the efficacy of immune cell-based therapeutics.


A549-RedFluc
Scaffold
luciferin
BLI monitoring

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Poster Presentation : **MAT.P-366**
Material Chemistry
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Advanced Full-Color Perovskite Nanocrystal Patterning for Ultrathin Skin-Attachable Displays with Ultrahigh-Resolution

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Advanced displays require high-resolution RGB pixels and flexible form factors for future applications. Here, we introduce a method for full-color ultrahigh-resolution patterning of perovskite nanocrystals (PeNCs) for skin-attachable ultrathin displays. The double-layer transfer printing involving PeNCs and organic layers used for charge transportation inhibits internal fracturing in the PeNC layer during fabrication. This approach enables the formation of RGB pixelated PeNC patterns with a resolution of 2,550 pixels per inch and monochromatic patterns with 33,000 line pairs per inch, achieving a transfer yield of 100%. The perovskite light-emitting diodes (PeLEDs) produced with active layers applied through transfer printing demonstrate high electroluminescence properties, with high external quantum efficiencies of 15.3% for red, 14.8% for green, and 2.5% for blue, respectively, surpassing those of previously reported printed PeLEDs. Moreover, the double-layer transfer printing technique facilitates the manufacturing of full-color thin PeLEDs capable of conforming to curved surfaces, such as human skin, while also enduring diverse mechanical stresses. These results emphasize the potential of PeLEDs for high-resolution full-color wearable displays.

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Poster Presentation : **MAT.P-367**

Material Chemistry

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On-sight Rapid Detection of Heavy Metal Ions in Environmental Wastewater: Towards Environmental Monitoring

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Heavy metal ions are widely utilized in various industries, including mining, metallurgy, agriculture, and manufacturing. However, at the end of these industrial processes, heavy metal ions come into the environment, causing risks to human health. Consumption of food and water contaminated with heavy metals is a common route of exposure. Seafood, vegetables grown in contaminated soil, and water from polluted sources can all contribute to heavy metal intake through ingestion. In this work, optical and rapid detection of heavy metal ions from the range of 20 different cations and anions (Al3+, Ca2+, Cd2+, Cl-, CO2+, Cu2+, Eu3+, Fe2+, Fe3+, HPO4-, I-, K+, Li+, Mg2+, Na2+, Ni2+, No3-, Pb2+, SO4- and Zn2+) was investigated. Carbon dots were synthesized via a simple and cost-effective hydrothermal method, resulting in fluorescent nanoparticles with excellent stability and biocompatibility. The synthesized carbon dots were characterized using various spectroscopic and microscopic techniques to elucidate their structural and optical properties. The results demonstrate selective and sensitive detection of the target metal ions Cd2+, Cu2+, and Pb2+ over a wide concentration range, with detection limits in the sub-ppm range. Furthermore, the sensing platform exhibits excellent stability and reproducibility, making it suitable for on-site applications in environmental monitoring.

Poster Presentation : **MAT.P-368**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Exploring ortho-Carborane-Substituted Anthracene Materials in Organic Light-Emitting Diodes Utilizing Hybridized Local and Charge Transfer Mechanisms

Won-Sik Han*, Jina Lee

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Two ortho-carborane-substituted anthracene derivatives incorporated with carbazole, PCAPCb and PCAMCb, were prepared. By manipulating the substituent at the ortho-carborane (o-Cb), we effectively modulated their photophysical and electrochemical properties. Introducing a phenyl group at the o-Cb resulted in dual emission in the solution state, facilitated by efficient charge transfer from carbazole to the o-Cb groups. Conversely, their methyl analogs exhibited distinct locally-excited emission. Particularly intriguing features were observed in their solid-state photochemistry. In film form, PCAPCb displayed multiple photoemissions, with predominant strong emission at 630 nm (CT emission) and weak emission at 420 nm (LE emission), whereas PCAMCb showed strong emission at 420 nm (LE emission) and weak emission at 640 nm (CT emission). This demonstrated that the CT states of o-Cb can be turned- on or -off. Even slight modifications in molecular geometries by altering substituents strongly influenced their excited-state properties and subsequent emission behaviors. To leverage the unique properties of PCAPCb and PCAMCb, we fabricated white OLED devices and examined their electroluminescence characteristics.

Poster Presentation : **MAT.P-369**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

High valence Mo-decorated NiFe-Layered Double Hydroxide as High Efficiency Catalyst for Oxygen Evolution Reaction on Near- Neutral pH Electrolyte

Il Ran Jung, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Although the electrolysis of water for hydrogen production has been considered as a crucial facet in renewable energy technology, it’s the sluggish kinetics of oxygen evolution reaction at the anodic electrode might limit the practical application of this technology. In alkaline electrolyte, NiFe-layered double hydroxide (LDH) has been recognized as potential OER catalyst. However, in less corrosion environment of neutral pH electrolyte, NiFe LDH still shows the poor OER performance due to its low conductivity and a limited number of active sites on the material surface.To overcome these challenges, the Mo-decorated NiFe-LDHs was synthesized through a facile immersion method and applied as OER catalyst in a near-neutral electrolyte (1M $KHCO_3$).The optimal Mo-decorated NiFe-LDH, featuring a well-defined nanosheet structure with the homogeneous distribution of high-valence Mo on the surface exhibits the remarkable OER catalytic activity in 1 M $KHCO_3$ with a low overpotential of 339 mV at current density of 10 mA cm^{-2} (η_{10}) and small tafel slope of 112 mV dec^{-1}, which is outstanding compared to pristine NiFe LDH (η_{10} = 364 mV and Tafel slope of 150 mV dec^{-1}). This results open the new approach in synthesis of advanced OER catalysts in near neutral pH electrolyte.

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Poster Presentation : **MAT.P-370**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhanced production of propanol through CO2 reduction reaction using self-assembled thiol monolayer on Cu catalyst.

Donghyeon Kim

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In the era of global warming, converting carbon dioxide into high value-added compounds through electrochemical catalysts is attracting attention. Among the CO2 reduction reaction (CO2RR) catalysts, Cu is a monometallic electrocatalyst specialized in the reduction of CO2 to C1-C2 product. Numerous studies have reported that hydrophobic surfaces in CO2RR can control selectivity towards C2 products. Among these, some researchers have reported that catalyst materials with high selectivity are obtained by attaching thiol groups to the catalysts to create hydrophobic surface. However, most research primarily focuses on suppressing the hydrogen evolution reaction (HER). Herein, thiol-Cu catalysts were fabricated by self-assembly in a thiol-containing solution. By varying the chain length of the alkyl thiol from 0 (pristine Cu) to 14 (tetradecanethiol), the selectivity of CO2 to propanol was tuned. As a result, the highest Faradaic efficiency (F.E.) was achieved with a monolayer of hexanethiol.

Poster Presentation : **MAT.P-371**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Montmorillonites with Inserted Organo-Metallic Complex: Breakthrough Electrolysis Catalysts for Enhanced Oxygen Evolution Reaction Performance.

In Seon Lee, Min Hyung Lee[1,*]

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In light of the urgent need to address fossil fuel depletion and the environmental crisis, there's a pressing demand for highly efficient and cost-effective energy sources. Water electrolysis has emerged as a promising avenue for producing green hydrogen, offering an environmentally friendly alternative. However, the sluggish kinetics of the oxygen evolution reaction (OER) at the anodic electrode presents a barrier to practical application. Hence, considerable efforts have been devoted to developing efficient OER electrocatalysts to minimize overpotential. This study introduces a novel approach to synthesizing OER electrochemical catalysts by inserting organo-metallic complexes of 1,10-Phenanthroline (Phen) with Ni, Co, and Fe into montmorillonite (MMT) clay layers. Analysis via X-ray diffraction and transmission electron microscopy confirms successful insertion of the organo-metallic complexes into the MMT clay layers, resulting in an expanded interlayer distance. Evaluation of the prepared samples for OER demonstrates that MMT:Co(Phen)2 exhibits superior OER performance, with an overpotential of 313 mV at a current density of 10 mA cm-2 and remarkable long-term stability exceeding 50 hours. These promising results underscore the potential of leveraging organo-metallic complexes in the synthesis of advanced electrocatalysts for the OER.

Poster Presentation : **MAT.P-372**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pyrene-based hybridized local- and charge-transfer (HLCT) emitters integrated with carbazole and imidazole for OLED applications

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‘‘Hot-exciton’’ materials exhibiting high-lying reverse intersystem crossing (hRISC) are promising candidates for organic light-emitting diode (OLED) materials owing to their improved exciton utilization efficiency and efficiency roll-off. To explore the relationship between structure and properties in pyrene-based materials, we synthesized two derivatives, namely, p-PyCzIz and m-PyCzIz, by altering the substitution position of carbazole and imidazole groups. Our goal is to induce hybridized local- and charge-transfer (HLCT) states where both localized excitation (LE) and charge transfer (CT) occur simultaneously by controlling the LE/CT ratio in the excited state. We systematically investigated the photophysical, electrochemical, and thermal properties of these compounds, supported by density functional theory (DFT) calculations. The steric hindrance resulting from the substitution position significantly affects their photophysical properties and solvatochromic emission spectra clearly demonstrated the HLCT character of the materials. Both p-PyCzIz and m-PyCzIz exhibited relatively high photoluminescence quantum yields (PLQY) of up to 69% and 80%, respectively, along with excellent thermal stability. Finally, we examined the electroluminescence properties of devices utilizing p-PyCzIz and m-PyCzIz.

Poster Presentation : **MAT.P-373**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Utilization of Metal–Organic Frameworks as Sacrificial Precursors for the Synthesis of Carbon-Based Bifunctional Electrocatalyst

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The Zn-air battery is recognized as an efficient energy storage device due to its high theoretical energy density, cost-effectiveness, environmental friendliness, and stability. Within the Zn-air battery, two catalytic reactions take place at the positive air-electrode surface: the oxygen evolution reaction (OER) during charging and the oxygen reduction reaction (ORR) during discharging. In previous studies, expensive noble metals such as Pt and Ru-based catalysts have been employed for efficient OER and ORR reactions, prompting the need for the development of new bifunctional catalysts as substitutes for Pt and Ru-based catalysts. In this study, we successfully synthesized N-doped carbon nanotube (CNT) grown on a composite of Ni and C (Ni/C) through the pyrolysis of a mixture comprising Ni metal-organic framework and melamine at various ratios and temperatures.Subsequently, these materials were applied as bifunctional catalysts for both OER and ORR. The optimal samples, synthesized at a ratio of 1:3 between Ni metal-organic framework and melamine, and at 800 °C, exhibited superior catalytic performance, demonstrating an overpotential of 328 mV at a current density of 10 mA cm-2 for OER and a saturated current density of -11.3 mA cm-2 for ORR in an alkaline solution. These promising results signify a novel approach to synthesizing bifunctional catalysts involving metal-carbon-based composites for the air electrode in Zn-air batteries.

Poster Presentation : **MAT.P-374**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Influence of hydrophobization on the surface properties of mesoporous TiO2

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Titanium dioxide (TiO2) has got a great attention in various fields such as catalysis, dye-sensitized solar cells (DSSCs), photochromic devices, sensor, and cosmetics, due to its differentiated advantages from the others: high band gap energy, high stability and catalytic activity, and non-toxicity. The photocatalytic activity of TiO2 has been considered to be determined by the crystalline phase, crystal size, and specific surface area. To improve the photocatalyic activity of TiO2, small size and high crystallinity of nanoparticles have been used. Mesoporous TiO2 has a large surface area because of its high surface to volume ratio, and so it should in principle have high photochemical sterilization, because of the improved access to the active sites of TiO2. The active site of TiO2 was originated from surface hydroxyl groups. In this study, we prepared mesoporous TiO2 for the purpose of its usages by surface modification with hexamethyldisilazane. Here, we controlled the surface hydrophobicity from hydrophobic TiO2 surface in order to activate or deactivate the TiO2 surface.

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Poster Presentation : **MAT.P-375**
Material Chemistry
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Optimizing Li-Ion Battery Electrode Manufacturing for Processes

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Lithium-ion batteries are an exciting technology that plays a key role in the trend towards renewable and sustainable industrial solutions for electrification. Lithium-ion batteries are widely used in automotive, energy storage, and electronics sectors thanks to their high energy, power density and long life cycle and are expected to see further growth in the coming years. However, when producing lithium-ion batteries, if the characteristics of the powder are not understood, various problems such as non-standard material production and process time delays occur. In this study, in order to operate the process more efficiently, the FT4 Powder Rheometer is used to determine the main characteristics of the cathode material, a core material of lithium-ion batteries, and to set powder quality standards. Among FT4's various methodologies, stability and variable flow rate test and permeability test were performed and compared on three types of powder batches. Stability and variable flow rate test showed that Batch 1 had the lowest specific energy, meaning that Batch 1 had the lowest friction between particles. The permeability test results showed that Batch 1 had the highest pressure drop value and low permeability. This was found to be consistent with the fact that Batch 1 had the most uniform particles and showed high packing efficiency in the actual process. As a result, anode materials can be produced more efficiently by setting the specific energy and pressure drop values of batch 1 as quality standards.

Poster Presentation : **MAT.P-376**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Responsive Thin-Film interference Color from Conjugated Polymers

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Dynamic colors that respond to environmental changes are of great interest for diverse areas of science and technology ranging from chemical and biological sensors to smart information display. Here, we demonstrate a multitude of responsive colors from a conjugated polymer film, arising from thin-film interference. This mechanism provides excellent control over the thin-film color by varying the film thickness, type of substrate, and degree of polaron population, and is generally applicable to various conjugated polymers for further color variation. Furthermore, multiple sets of responsive colors are realized from a single polymer layer by patterning the underlying substrate to spatially modify the interference conditions. Using this system, we demonstrate reversible color changes induced by oxidative or reductive environment with color responsivity controllable with the nature of the polaron state.

Poster Presentation : **MAT.P-377**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Low-Toxic Quantum Dot Based Infrared Photodetector

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Infrared optoelectronic applications are attracting much attention in the application field these days. Especially artificial atoms, quantum dots, are showing a new era of optoelectronic application due to the unique tunability of the optical feature. Thanks to the quantum confinement effect and the recent development of the synthetic technique, low-toxic quantum dots are newly realized and expanding to wider optical regions. This poster will comprehensively present the newly developed candidate quantum dots, indium antimonide and silver telluride, from a new synthetic method to diode device fabrication. Surprisingly, both devices showed an outstanding performance, resulting in external quantum efficiency of 75% at 1250 nm and 16% at 1750 nm, respectively. As from the previous result, the surface of the quantum dots is shown to be critical to the stability of the dots after the ligand exchange. This poster will discuss the optical properties of pristine and ligand-exchanged dots and the synthetical method affecting the device's overall performance.

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The transformation from intraband transition to localized surface plasmon resonance of self-doped Ag_2Se colloidal quantum dots.

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The self-doped semiconductor nanocrystals can increase the carrier density, gradually combining localized surface plasmon resonances (LSPR) and the discrete energy. In this work, we present the optical property transformation from the excitonic transition to the LSPRs with an increase of carrier density in the Ag_2Se CQDs. As the nanocrystal growth time increases, the broad single absorption peak splits into two distinct peaks with different bandwidths. The splitting of the intraband transition mainly results from the asymmetrical crystal structure of the tetragonal Ag_2Se CQDs and becomes distinct when the nanocrystal changes its crystal structure from the cubic to the tetragonal structure. Additionally, after the surface plasmon resonance term is added to the k·p model, it distinctly fits the experimental data. This indicates that the peak contains LSPR characteristics and that the transitions within the mid-IR region are mixed with the LSPR of self-doped Ag_2Se quantum dots. As the nanocrystal growth time increases, the LSPR property increments and the excitonic transition in the mid-IR region decreases so that the intensity of MWIR emission declines.

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Poster Presentation : **MAT.P-379**
Material Chemistry
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Room Temperature Synthesis of Self-Doped Silver SelenideQuantum Dots Sensitive to Mid-infrared Light

So Young Eom, Jin Hyeok Lee, Haemin Song, Minhaeng Cho, Kwang Seob Jeong[*]

Department of Chemistry, Korea University, Korea

Self-doped silver selenide colloidal quantum dots (CQDs) that harness intraband transition as a major electronic transition in steady-state have emerged as an alternative midinfrared (IR)-sensitive material to Pb or Hg-based CQDs. Comparable to the previously reported hot-injection and cation-exchange methods for the self-doped Ag_2Se CQDs synthesis, a facile synthesis method of the self-doped Ag_xSe ($x \geq 2$) CQDs is reported that does not require high reaction temperature, reduces the cost of material synthesis, and enables widespread use of the self-doped nontoxic CQDs in various environments and applications. Through careful investigation of the crystal structure, compositional analysis, mid-IR absorption, photoluminescence, and photocurrent response, we demonstrate that the as-synthesized Ag_xSe CQDs exhibit peculiar optical and electrical properties of the self-doped CQDs, potentially highlighting their application as IR-active materials for mid-IR-based optoelectronics.

Poster Presentation : **MAT.P-380**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Ag-In-Ga-S Quantum Dots with Narrow Photoluminescence by Gallium ion Incorporation

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Heavy metal-free Ⅰ-Ⅲ-IV$_2$ based colloidal quantum dots (CQDs) have gained interest because of their wide wavelength-tunability, large absorption coefficients, and low toxicity which can substitute heavy metal-based colloidal quantum dots like CdSe, HgSe. However, it has been challenging to synthesize high color purity Ⅰ-Ⅲ-Ⅵ2 CQDs because broad photoluminescence (PL) feature arises from defects. So, we present one-pot synthesis method of a quaternary silver indium gallium sulfide (AIGS) CQDs exhibiting a narrow bandgap photoluminescence (PL). Synthetic condition analysis revealed that the foremost emission mechanism is highly sensitive to the degree of Ga incorporation into the CQDs. Ga atoms penetrated AIGS CQDs from the surface to the core by varying the reaction temperature and broad trap emission was gradually suppressed, while band-edge emission was intensified. With such a narrow PL peak, we further studied the ZnS shell growth achieving PLQY of 16 % and fabricated light-emitting diodes through AIGS/ZnS CQDs. This investment about the change of Ga ions in the AIGS CQDs and formation of core-shell structure with less lattice mismatch would enable future applications for the non-toxic-QLED and other optoelectronic devices.

Poster Presentation : **MAT.P-381**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Extended short-wavelength infrared photoluminescence of nonstoichiometric silver telluride colloidal nanocrystals

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The demand for non-toxic nanomaterials in the short-wavelength infrared (SWIR) range has increased over the past ten years. In this report, we introduce nonstoichiometric silver chalcogenide nanocrystals of Ag_xTe (where x > 2) and Ag_2Te/Ag_2S CQDs, which have a tunable bandgap across the SWIR region. By varying the atomic percentage of the metal and chalcogenide elements, we were able to successfully extend the emission frequency of the excitonic peak to 2.7 μm. The Ag_2S shell growth over the Ag_2Te core improved the emission intensity and structural rigidity, preventing crystal morphology deformation under the electron beam. We carefully studied the origin of the enhancement in the emission intensity and air stability of Ag_xTe and Ag_2Te/Ag_2S CQDs through X-ray photoelectron spectroscopy (XPS). The optical properties and infrared photocurrent of Ag_xTe CQDs will provide new opportunities for solution-based SWIR applications.

Poster Presentation : **MAT.P-382**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Quantum Plasmon Resonance of Ag2Se Nanocrystals with Ultranarrow Bandwidth in Mid-Infrared Region

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The quantum plasmon resonance (QPR) could lead to the novel physical and optical features due to its combined properties of classical and quantum properties. However, the research has been restricted from the challenges of increasing the electron concentration of semiconductor nanocrystals (NCs). Here, we demonstrate the QPR of a Ag2Se NC in mid-infrared region by self-doping. The Ag2Se NCs become highly self-doped due to the weakened quantum confinement effect as the diameter of the NCs grow larger by passivating the NC surface with chloride ligand. The QPR feature was analyzed by infrared spectroscopy, ultraviolet photoelectron spectroscopy, and the photoluminescence spectroscopy. Two theoretical models that combined the characteristics of the metal and semiconductor were developed for the analysis, which revealed the QPR coupling with the intraband transition and the limited nature of electron density in semiconductor NCs. The QPR characteristics decrease the peak bandwidth to 19.7 meV, which results in the long LSPR dephasing time. This demonstrates that the self-doped Ag2Se NCs could be an excellent platform material for investigating metal-semiconductor hybrid properties.

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Midwavelength Infrared Tellurium Nanowire Laser

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Recently, Midwavelength infrared (MWIR) active nanomaterials have attracted much interest because of their optical properties such as excellent transmission in atmospheric windows, which can be used for unmanned vehicle communication and telecommunication and bio-imaging. Tellurium (Te) is a narrow-band-gap semiconductor, has shown the potential of non-toxic MWIR emitter, while the research has been focused on epitaxial growth and other properties. Here, we report the first MWIR lasing of the solution-phase Te nanowire laser ensemble at 3.6 μm, exhibiting strong MWIR photoluminescence (PL) at room temperature and MWIR lasing below 129 K that had never been observed in colloidal nanomaterials before. The fwhm of the emission peak becomes larger and narrower and the center peak red shifts by ~100 cm^{-1} with a decrease in temperature. Also, other weak emission peaks appear at double and triple frequency as the temperature decreased which are the second-harmonic field and third-harmonic field due to the unique structure of the tellurium nanowire. It can expand the range of the infrared lasing frequency up to the near infrared range. MWIR lasing has been clearly observed from Te nanowires embedded in a human neuroblastoma cell, which could further realize deep-tissue imaging and thermotherapy in the near future.

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Material Chemistry

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Expansion of the Photodetection Range Through the Cation Exchange Method

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Rather than relying exclusively on heavy metal-based mid-infrared active materials, researchers have increasingly turned their attention to silver selenide colloidal quantum dots (CQDs) as potential alternatives, which demonstrate steady-state intraband transitions between $1S_e$ and $1P_e$ states. Nonetheless, expanding these intraband transitions to higher energy states presents a notable challenge, as they are currently confined to the mid-IR wavelength range. In this work, we introduce cation-exchanged Ag_xSe (X>2) CQDs derived from PbSe CQDs, showcasing intraband transitions up to 0.39 eV. Through applications in electrochemical luminescence and intraband photodetectors, we have confirmed the presence of steady-state intraband transitions in cation-exchanged CQDs. I-V characteristics and on-off infrared photocurrent were measured across different device structures and temperatures. This research highlights the potential of the cation exchange method in broadening the range of intraband transitions. The expanded spectral range of Ag_xSe CQDs further improves their suitability for infrared detection applications.

Poster Presentation : **MAT.P-385**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

A hydrophilic Janus-faced separator with functionalized nanocarbon for stable cycling of aqueous Zn-metal batteries

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Aqueous zinc (Zn) metal batteries (AZBs) are one of the promising candidates for post-Li-ion batteries for cost-effective and safe large-scale energy storage systems. However, the irreversibility of the Zn metal anode (ZMA) due to Zn dendrite growth and “dead Zn” formation, which is an electrically isolated Zn particle, is a crucial issue for the practical use of AZBs. In response to these drawbacks, a Janus-faced separator composed of an acid-treated carbon supportive layer (aCSL) is proposed, which can perform various functions, rendering additional reaction sites for Zn deposition/dissolution and uniform Zn2+ ion flux owing to excellent wetting by endowed hydrophilicity. By manipulating current density and Zn plating capacity, hydrogen evolution reaction (HER)-dominant and HER-minimized protocols for Zn coulombic efficiency (CE) are proposed for assessing the Zn reversibility. Remarkably, the aCSL exhibits the highest initial CE of each newly suggested protocol, which indicates that the aCSL can suppress the water-induced side reactions and achieved an excellent CE of 99.6%(@ 1 mA cm−2) during 900 cycles and stable symmetric cell performance over 1200 hours(@ 1 mA cm−2). Due to these interesting features, the Zn‖α-MnO2/CNT full cell shows stable cycle performance with capacity retention of 61.3% during 2000 cycles.

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Elucidating critical origin for capacity fading in High-voltage coin cell with FSI-based electrolyte

Byung Gon Kim

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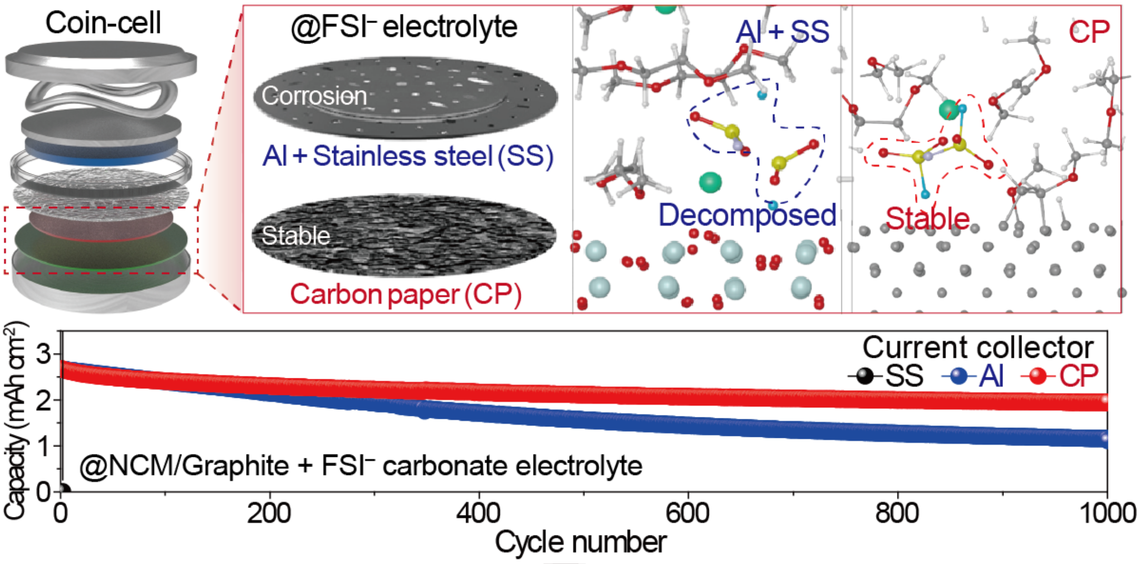
F-containing functional electrolytes have been extensively investigated to improve the performance of Li-metal batteries as they generate stable LiF-based solid–electrolyte interphase layers, improving Li deposition/dissolution efficiency. However, these imide-based electrolytes corrode not only the Al current collector but also the stainless steel (SS) component of the coin cell at high operating voltages. Additionally, deciding upon which part of the corrosion has a greater effect on the performance degradation remains a topic of debate. In this study, through systematic cell design exposing SS to LiFSI-based electrolyte, it is found that SS corrosion is a more dominant cause of capacity fading than the Al case. Moreover, the computational study reveals that the electron transfer from Al to SS decomposes FSI– and the resulting byproducts finally corrode Al. To develop stable cells by removing corrosion factors, the SS and Al-free pouch-type cells are proposed by integrating carbon current collectors and locally high-concentration electrolyte and exhibit 430 cycles with a coulombic efficiency of 99.93%. This study demonstrates the importance of careful selection of cell components and systematic cell design to ensure a robust interface at the cathode side, suggesting the necessity to develop a new testing cell to replace the current coin-cell platform.


Coin-cell
@FSI⁻ electrolyte
Corrosion
Al + Stainless steel (SS)
Stable
Carbon paper (CP)
Al + SS
Decomposed
CP
Stable
Capacity (mAh cm⁻²)
3
2
1
0
Current collector
SS
Al
CP
@NCM/Graphite + FSI⁻ carbonate electrolyte
0
200
400
600
800
1000
Cycle number

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Material Chemistry

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Facile synthesis of molybdenum carbide nanoparticles stabilized in mesoporous three-dimensional (3D) graphene and its characterization

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In the field of renewable energy, a surge in development to create clean energy technology is exploding, because of the shortage of fossil fuels and environmental pollution. Therefore, technologies such as electrolysis to produce clean hydrogen fuel and energy storage systems for renewable energy have become important research areas. In recent years, transition metal carbides (TMCs) have gained major attention due to their characteristics such as high electrical conductivity and excellent chemical stability, thus intense research has been studied on TMCs as promising candidates for electrocatalysts. Especially, the molybdenum carbide is considered an alternative catalyst for electrochemical applications including hydrogen evolution reaction (HER) since it has outstanding HER activity and remarkable stability. To obtain the molybdenum carbides, the existing synthesis procedures are solid-gas reaction, chemical vapor deposition, sonochemical synthesis, and DC arc charge plasma synthesis. However, these processes often have complex steps, using harmful chemicals, or demanding high energy consumption. In this report, we demonstrate the facile synthesis method of molybdenum carbide nanoparticles incorporated in mesoporous graphene via a simple carburization process. The structural, morphological, and porous characteristics of the obtained sample were investigated in detail.

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Material Chemistry

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2D Lepidocrocite-type layered titanate coated on carbon felt as the negative electrode for high-performance vanadium redox flow battery

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Vanadium redox flow battery (VRFB) is regarded as the most promising candidate for grid-connected energy storage systems due to its flexible design, thermal safety, and deep discharge capacity. However, its performance is limited by the irreversible hydrogen evolution reactions (HER) on the surface of the negative electrode that competes with the desired V^{3+}/V^{2+} redox couple reactions. The HER consumes current, corrodes the electrode, decreasing the active electrochemical surface area, and overall causing overpotential and efficiency loss. For the first time, we have fabrication the lepidocrocite-type layered titanate nanosheets ($Ti_{1.83}\square_{0.17}O_{4-x}$; □ = vacancy, $x = 0.67$) modified carbon felt (LTNS@CF) and evaluated its performance as the negative electrode for VRFB. The LTNS@CF electrode was prepared by coating an extremely small amount (~0.0043 wt. %) of chemically exfoliated LTNS stable colloidal suspension on pristine carbon felt (P-CF) using the dip-withdraw-dry method. Notably, the LTNS achieved a high specific discharge capacity of 7.32 Ah L^{-1} at 200 mA cm^{-2}, which is ~254 % higher than that of bare P-CF (2.07 Ah L^{-1}). P-CF failed beyond 200 mA cm^{-2} while the LTNS@CF proceeded to record high energy efficiencies at 225, 250, 275, and 300 mA cm^{-2}. The superior electrochemical performance of LTNS@CF electrode arises from the desired properties of the coated layered titanate, including the 2D anisotropic shape that causes firm adhesion to the P-CF substrate, the negative charge that provides electrostatic reaction sites for the positively charged vanadium ions, corrosion resistance of Ti-O covalent bond in the acidic electrolyte, and its hydrophilicity that enhances the wettability of the electrode.

Poster Presentation : **MAT.P-389**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pre- and Post-Hydrothermal Modification of Mesoporous Graphene /Exfoliated Layered δ-MnO2 for Enhanced Supercapacitor Performance

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This study presents an innovative dual-strategy approach aimed at enhancing the capacitive performance and electrical characteristics of electrode materials for electrochemical energy storage systems. Two hybrid materials, MG/δ-MnO2 and MG/Mn3O4, tailored specifically for supercapacitor electrodes, are investigated. Through meticulously controlled post-hydrothermal treatments, exfoliated layered δ-MnO2 is transformed into Mn3O4, respectively. The resulting hybrids exhibit hierarchical nanostructures characterized by unique mesoporous networks, elevated surface area, and enhanced electrical conductivity facilitated by graphene p-doping via electron transforming to manganese oxide. As supercapacitor electrodes, the optimized MG/Mn3O4 demonstrates a remarkable specific capacitance of 1167 F/g at a current density of 1.0 A/g, showcasing exceptional rate performance and outstanding cycling stability over 10,000 charge-discharge cycles while retaining 71% capacitance. This study underscores the significance of designing layered transition metal oxide hybrid with mesoporous graphene (MG) networks to advance energy storage and conversion technologies.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **MAT.P-390**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Nanostructured NiTe on Mesoporous Graphene for enhanced Electrocatalytic Oxygen Evolution Reaction

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The electrocatalytic oxygen evolution reaction (OER) is a crucial step in various electrochemical energy devices, including water electrolyzers, metal-air batteries, and fuel cells. However, the sluggish kinetics of the OER reactions hinder their widespread application. To address this challenge, we synthesized NiTe-loaded mesoporous graphene (MG) nanohybrids via in-situ growth on the surface of MG, with varying nominal weight percentages of NiTe (5%, 10%, and 15%). Diverse structural and morphological analyses confirmed the successful synthesis of hexagonally structured NiTe within the MG nanohybrids. The wrinkled 3D mesoporous graphene scaffold facilitated the attachment and dispersion of NiTe nanoparticles, preventing agglomeration. The optimized composition of NiTe-10 wt%/MG nanohybrid electrocatalyst demonstrated superior OER activity, with a small overpotential of 240 mV at 10 mA cm−2, a low Tafel slope of 52.8 mV dec−1, and sustained the OER stability over an extended duration in 1 M KOH (pH=14) electrolyte. Combining NiTe and MG into a nanohybrid material resulted in a synergistic effect, enhancing the concentration of active species that modulated the electronic structure, leading to a lower energy barrier and improved OER activity. This work demonstrates a novel nanohybrid approach for OER electrocatalysts, enhancing both efficiency and stability, paving the way for improved energy conversion technologies.

Poster Presentation : **MAT.P-391**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Pt doped porous In_2O_3 nanoparticle structures-Based Hydrogen sensor

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This study fabricated Pt-loaded porous In_2O_3 sensors using a simple microwave synthesis method and electroless plating and investigated their hydrogen sensing characteristics. In particular, the 3.8at% Pt-loaded In_2O_3 NPs sensor exhibited high gas sensitivity to hydrogen compared to interfering gases at 150°C for 5 ppm hydrogen. This is attributed to efficient reaction between Pt nanoparticles loaded on the surface of porous In_2O_3 nanoparticles and hydrogen. Therefore, the results of this study are expected to contribute to the development of high-performance sensors for low-concentration hydrogen detection in the future, thereby contributing to the cyclic hydrogen energy field.

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Poster Presentation : **MAT.P-392**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Comparative study on adsorptive removal of radioactive Cs^+ ions from aqueous solution by raw white and acid-activated white clay

Keon Sang Ryoo

Department of Chemical and Biological Engineering, Andong National University, Korea

Raw white clay was treated with H_2SO_4 (6 M) at 80oC for 6 h under mechanical stirring, and the resulting acid-activated clay was used as an adsorbent for the removal of Cs^+ ion in aqueous solution. The characteristics of raw white clay and acid-activated white clay were observed by X-ray Fluorescence Spectroscopy (XRF), Energy Dispersive X-ray Spectroscopy (EDX), and BET Surface Area Analyzer. While activating raw white clay with acid, cations such as Al^{3+}, Ca^{2+}, Mg^{2+} and Fe^{3+} are partially eluted from the crystal lattice of clay, and lead to the increase in the surface area and the pore volume through the opening of lattice. The surface area and the pore volume of acid-activated white clay were found to be roughly three times higher than raw white clay. Generally, removal efficiency of Cs^+ ion by acid-activated white clay showed much higher compared with raw white clay. At 50 mg L^- of Cs^+ ion concentration and 1 g of dose, the removal efficiency of Cs^+ ion by raw white clay and acid-activated white clay were 57.5 % and 96.9%, respectively. The data obtained from this study were fitted to the adsorption isotherm and the kinetic model, respectively. It revealed that the Langmuir isotherm and the pseudo-second-order kinetic model describes well the adsorption behavior of Cs^+ on both raw white clay and acid-activated white clay owing to the higher correlation coefficient R^2. Based on the Langmuir isotherm coefficient Q, adsorption capacity of Cs^+ ion by raw white clay and acid activated clay were 5.65 mg g^{-1} and 10.6 mg g^{-1}, respectively. The results demonstrated that clay activated with acid treatment can be used as more effective adsorbent for the removal of Cs^+ from aqueous solution than raw clay.

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Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Comparative study for adsorptive removal of radioactive Cs^{+}, Sr^{2+} and Co^{2+} ions from aqueous solution by acid-activated white clay

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Raw white clay was acidified with H_2SO_4 (2 M) and then activated in a furnace for 2 hr at 150 oC. The resulting acid-activated clay product was used as an adsorbent for the removal of radioactive substances such as Cs^{+}, Sr^{2+} and Co^{2+} ions in aqueous solution. The physicochemical characteristics of raw white clay and acid-activated clay were determined by X-ray Fluorescence Spectroscopy (XRF), BET Surface Area Analyzer and Energy Dispersive X-ray Spectroscopy (EDX). While activating raw white clay with acid, the part of Al_2O_3, CaO, MgO, SO_3 and Fe_2O_3 consisting of raw white clay was eluted from the lattice, resulting in the increase in the specific surface area and the pore volume as well as adsorption active sites. The specific surface area and the pore volume of acid-activated clay were three times higher compared to raw white clay. Applicability of acid-activated clay for Cs^{+}, Sr^{2+} and Co^{2+} ions removal was performed in a batch mode. The fast adsorption of Cs^{+} and Sr^{2+} relative to Co^{2+} on acid-activated clay took placed in the first few minutes and equilibrium was reached within about 10 min. The effects of initial concentrations and dosage on adsorption capacity of Cs^{+}, Sr^{2+} and Co^{2+} ions were investigated. At 100 mg L^{-} of initial concentration and 1.0 g of dosage, removal efficiencies of Cs^{+}, Sr^{2+} and Co^{2+} ions showed 60.0 %, 27.3 %, and 88.1 %, respectively. The experimental adsorption data were fitted to the adsorption isotherm and kinetic models. It was found that the Langmuir isotherm was described well to the adsorption behavior of Cs^{+}, Sr^{2+} and Co^{2+} ions on acid-activated clay rather than Freundlich isotherm. The Langmuir isotherm constant (Q) for Cs^{+}, Sr^{2+} and Co^{2+} ions was found to be 8.81, 3.78 and 10.20 mg g^{-1}, respectively. Compared to the pseudo-first-order kinetic model, the pseudo-second-order kinetic model was more suitable for adsorption of Cs^{+}, Sr^{2+} and Co^{2+} ions in water/acid-activated

clay medium owing to the higher correlation coefficient (R2) and the more proximity value of the experimental value qe,exp and the calculated value qe,cal.

Poster Presentation : **MAT.P-394**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Recovery of Co, Ni, and Mn from spent lithium-ion secondary batteries using lactic acid and oxalic acid as leaching and precipitation agents

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In this study, the cathode active material was first separated from the aluminum foil through a heat treatment at 500oC. The separated cathode active material was calcined at a temperature of 1000oC to remove completely carbon particles generated from the organic adhesive during heat treatment. And then, Co, Mn, and Ni were recovered from the cathode active material using lactic acid and oxalic acid as leaching and precipitating reagents. The lactic acid showed almost similar metal leaching effects from cathode active material compared to sulfuric acid, hydrochloric acid, and nitric acid. The optimal metal leaching efficiency by lactic acid was obtained when 30 g of the cathode active material was added to the 2 N lactic acid solution. At these conditions, the leaching efficiencies of Li, Mn, Co, and Ni were 93.4%, 92.2%, 95.2%, 94.8 %, respectively. Subsequently, when 5 g of oxalic acid was added to the lactic leachate of 2 N, a phenomenon in which all metals were precipitated was observed. Based on this result, the optimal condition for precipitating the leached metals using oxalic acid was oxalic acid : cathode active material = 1 : 7 (w/w %). Through XRD and EDX analysis, the precipitate was identified as a polynuclear crystalline material in which the three components of Mn, Co, Ni oxalates were mixed with approximately 7 : 4 : 10 in integer ratio of weight. The produced precipitate can be recycled as raw material of cathode active material through simple heat treatment and the addition of lithium source.

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Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Assessment on the magnesia/mineral supplier-treated Korean cattle compost (MMC) for the reduction of water pollution and the recovery of soil through field test

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Background: The soil in North Gyeongsang Province in Korea is mostly made up of sand, which lacks various essential minerals for growing crops, and also increases the pollution of the surrounding water when it rains. Therefore, in order to solve the above problem, the applicability of water pollution reduction and soil restoration was examined by using compost prepared by mixing MgO and mineral sources in a weight ratio of 1:2 with the existing Korean beef compost. Method: MgO used is a powder obtained by activating MgCO3 natural stone at 800°C for 2 hours, and the mineral source was made by adding white soil to a sulfuric acid solution and heating it at 80°C for 1 hour and then recovering the sulfuric acid solution. After spraying the newly prepared compost on 20 farmland, water pollution and soil fertility were measured through analysis of water and soil items such as TOC, BOD, T-N, T-C, and EC before and after spraying.Significant findings: When newly prepared compost was applied to the soil, the concentrations of TOC, BOD, T-N, and TP were reduced by 19.09%, 28.0%, 30.9%, and 27.5%, respectively, compared to commercial compost. On the basis of these results, it was confirmed that newly prepared compost is better than commercial compost for the water pollution reduction effect and the inhibition of green algae generation. Through soil analysis, the levels of EC and effective phosphoric acid in the soil were lower in the newly prepared compost than in the commercial compost. It is expected that soil fertility can be increased by reducing the rate of nutrient loss caused by rainfall.

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Poster Presentation : **MAT.P-396**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhanced Biocompatibility of Dexamethasone through Hybridization with 2D Inorganic Materials for Drug Delivery

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Dexamethasone (DEX) is a glucocorticoid with anti-inflammatory effects. It can be used for various diseases such as autoimmune diseases, allergies, cancer, ophthalmic diseases and COVID-19, etc. However, its efficacy is hindered by poor water solubility, necessitating higher dosages that may lead to adverse effects, including hypertension, peptic ulcers, hyperglycemia, and Cushing's syndrome. To overcome these limitations, we focused on developing a drug delivery system using layered double hydroxide (LDH) as a carrier to enhance the therapeutic efficacy of DEX. Employing co-precipitation, ion-exchange, and exfoliation and reassembling methods, we successfully intercalated DEX into the interlayer spaces of LDH. X-ray diffraction, molecular spectroscopy, and thermogravimetry analyses revealed the stabilization of DEX molecules within LDH interlayer spaces through electrostatic interactions, preserving their functionality and structural integrity. SEM and DLS results showed that the DEX-LDH particles were evenly dispersed with uniform size. Sustained release properties of DEX under various pH conditions were explored for potential application in the tumor microenvironment. Furthermore, biocompatibility and efficacy of the nanohybrids were evaluated through MTT assays using mouse fibroblast cells and breast cancer cells, respectively, demonstrating their suitability for medical applications. In conclusion, the DEX-LDH nanohybrid exhibited superior efficacy and improved distribution compared to DEX alone and has the potential to enhance therapeutic efficacy.

Poster Presentation : **MAT.P-397**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Enhancing Ascorbic Acid Stability with Precision Fabrication of 2D/3D Inorganic/Organic Nanohybrids

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Ascorbic acid (AA) is an essential nutrient crucial for human metabolic processes and physiological functions. However, its efficacy is limited due to easy oxidation and decomposition when exposed to the atmosphere. This study aimed to develop a stable AA preparation suitable for prolonged use under physiological conditions. To achieve this, we synthesized AA-zinc basic salt (ZBS) nanohybrids through co-precipitation, incorporating AA into the ZBS layer. We demonstrated the change from 2D to 3D structures of the AA-nanohybrids according to the concentration of ethanol in the solvent, as confirmed by Fourier transform infrared spectroscopy (FT-IR) and X-ray diffraction (XRD) analyses. Nanohybrid structure manipulation allowed the modulation of AA content, as shown by ultraviolet-visible (UV-Vis) spectroscopy. Furthermore, 3D AA-nanohybrids were confirmed to have a high specific surface area using the Brunauer–Emmett–Teller (BET) method. These AA-nanohybrids exhibited negligible cytotoxicity towards fibroblasts but demonstrated significant cytotoxicity against human melanoma and epidermoid carcinoma cells. The results indicate that AA-nanohybrids can effectively protect AA against oxidation and degradation, showing promising potential for diverse biomedical applications, particularly in drug delivery systems.

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Poster Presentation : **MAT.P-398**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Caffeic Acid-Layered Double Hydroxide Nanohybirds with Improved UV Protection for Cosmetic Applications

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Caffeic acid (CA), a component derived from plants, possesses not only antioxidant capabilities but also UV-shielding functionality. However, it has been reported that CA exhibits low stability when exposed to UV irradiation and oxygen. To overcome these limitations and enhance UV-shielding efficacy, we have developed a novel drug delivery system by incorporating CA into 2D-layered double hydroxides (LDHs) to form the nanobyrids. LDHs are well-known for excellent drug delivery carriers, serving as biocompatible host matrix capable of encapsulating various anionic molecules into their interlayer spaces. We synthesized CA-LDH nanohybrids by intercalating CA into the interlayer spaces of LDHs via co-precipitation, ion exchange, and exfoliation-reassembly methods. CA-LDH synthesized using the ion exchange method indicated that successful intercalation of CA into the interlayer spaces of LDH and greatest crystallinity in XRD analysis. The plate-like morphology and particle size remained consistent after CA intercalation, as observed through FE-SEM and DLS analyses. The CA contents in CA-LDH nanohybrids were determined at 325 nm using UV-Vis spectroscopy. The UV-shielding performance of CA-LDH nanohybrids exceeded that of pure CA and even commercially available ZnO and TiO2. Furthermore, CA-LDH nanohybrids also addressed the issue of white cast commonly associated with ZnO and TiO2. The present CA-LDH nanohybrids could provide a promising UVA and UVB blocking agent for cosmetic applications.

Poster Presentation : **MAT.P-399**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Strategies for Targeted Boron Neutron Capture Therapy using 10Boron Drug-Layered Double Hydroxide Nanohybrids

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The present study investigates the utilization of layered double hydroxide (LDH) as a two-dimensional carrier for delivering 10boron in boron neutron capture therapy (BNCT). In order to achieve an effective therapeutic effect in BNCT, it is necessary to selectively accumulate a sufficient amount of 10B in tumor cells from agents containing 10B. To meet these requirements, we incorporated two clinically used 10B drugs, 4-Borono-L-phenylalanine (BPA) and sodium mercaptoundecahydro-closo-dodecaborate (BSH), into LDH to form the nanohybrids. The synthesized nanohybrids were subsequently coated with bovine serum albumin (BSA) to prevent aggregation and improve biocompatibility. X-ray diffraction patterns were used to determine the d-values of the BPA-LDH and BSH-LDH nanohybrids, which were found to be 1.59 nm and 1.16 nm, respectively, indicating successful intercalation of BPA and BSH molecules into the interlayer space of LDH. The synthesized nanohybrids were characterized via ICP analysis to confirm their chemical composition. SEM and DLS analyses revealed uniform dispersion of both nanohybrids in terms of size. The feasibility of BNCT was confirmed through an in vivo experiment conducted in collaboration with the Kyoto University Research Reactor Institute. In conclusion, the combination of BNCT with the 10B delivery system utilizing LDH holds great promise as an targeted therapeutic platform for cancer treatment.

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Poster Presentation : **MAT.P-400**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Evaluating pre-clinical efficacy of 2D-biohybrid nanoparticles for Triple negative breast cancer therapy

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Triple-negative breast cancer (TNBC) remains challenging till date and it accounts for ~ 10-20 % of breast cancer incidents world wide without having any specific therapeutic regimens owing to the absence of three major receptors, HER-2, ER (estrogen receptor), and PR (progesterone receptor), which are typically observed in "normal" breast cancers. Therefore, novel treatment options such as combinatorial ones are important for TNBC. Here we used chemo and photo thermal therapies in single nanoparticle system as 2D bio-hybrid nanomaterials consisting of natural Phyto and human proteins such as Zein and Bovine serum albumin (BSA). To impart photo thermal effect (PTT), a dye known as IR-780 was introduced, whereas curcumin (CRC) was introduced to have chemo effect. Such a multi-faceted hybrid system showed optimal particle size, controlled release along with simultaneous PTT for effective TNBC therapy. These preliminary results suggested that the newly developed 2D-hybrid drug would be advantageous for treating TNBC and other subtypes of breast cancers effectively.

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Poster Presentation : **MAT.P-401**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Bifunctional Urea–Polyethyleneimine-Mediated Surface Engineering in tin oxide Electron-Transport Layer for Efficient and Stable Organic Solar Cells

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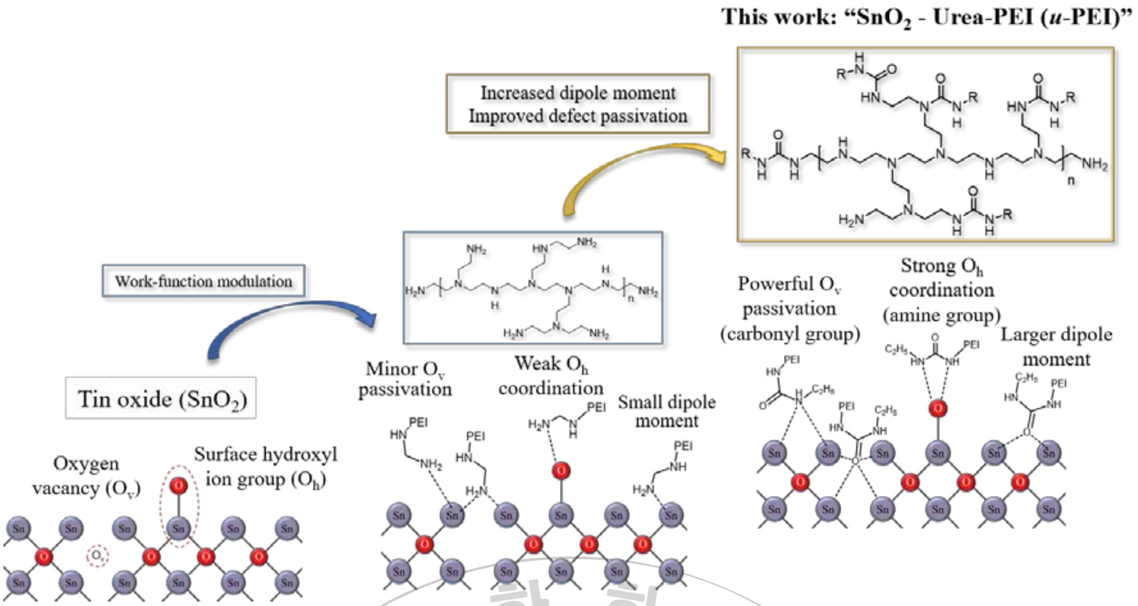
Because of its high conductivity, wide bandgap, and excellent photostability, tin oxide has long been recognized as an electron-transport layer (ETL) in organic solar cells (OSCs). However, the energy-level mismatch between the work function (WF) of tin oxide and the lowest unoccupied molecular orbital level of Y-series nonfullerene acceptors (NFAs), along with the abundance of surface defects on tin oxide, have limited its widespread application as ETLs in OSCs. Herein, a novel approach utilizing urea-functionalized polyethyleneimine (PEI) materials called u-PEIs for modifying tin oxide is introduced. This modification, which serves dual purposes of WF modulation and surface-defect passivation, can mitigate the energy barriers of tin oxide/Y-series NFA and increase the conductivity of the tin oxide film. PM6:Y6-based OSCs with u-PEI-modified tin oxide ETLs exhibit a remarkable efficiency of 16%, which significantly exceeds that (13.5%) achieved with bare SnO2-based OSCs, along with outstanding photo- and thermal- stability. This study confirms the efficacy of urea-functionalized PEI for efficient and stable OCSs, paving the way for tin oxide applications.


This work: "SnO₂ - Urea-PEI (u-PEI)"
Increased dipole moment
Improved defect passivation
Work-function modulation
Tin oxide (SnO₂)
Oxygen vacancy (Oᵥ)
Surface hydroxyl ion group (Oₕ)
Minor Oᵥ passivation
Weak Oₕ coordination
Small dipole moment
Powerful Oᵥ passivation (carbonyl group)
Strong Oₕ coordination (amine group)
Larger dipole moment
Sn
O
PEI
n

Poster Presentation : **MAT.P-402**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Shape-Controlled Hydrothermal Synthesis of $ZnCo_2O_4$ nanostructures

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$ZnCo_2O_4$ that has excellent electrochemical performance is promising materials for catalyst, lithium ion batteries, supercapacitors. In this work, $ZnCo_2O_4$ was synthesized by reflux system. The samples were controlled into various shapes by adding Hexamethylenediamine(HMT), urea, NH_4F and adjusting the ratio of water and ethylene glycol(EG) as solvent. The structural properties of the $ZnCo_2O_4$ were analyzed by using SEM, XRD, raman spectra. The morphologies of these samples were identified as sheet, sphere and spindle shapes by SEM. the samples annealed at 350℃ were fabricated with cubic spinel $ZnCo_2O_4$ regardless of shape. This work confirmed that $ZnCo_2O_4$ can be controlled into various shapes by using additives.

Poster Presentation : **MAT.P-403**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Low-temperature hydrocracking of LDPE over acidic Catalysts

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Plastic has become an essential part of the modern lifestyle due to its wide application in many sectors (transportation, construction, and packaging, medical, cosmetic)1. The exponential increase in global plastic production is anticipated to increase plastic pollution. Diverse recycling solutions have been proposed to address the issues with waste plastic, but they face significant economical and technical hurdles2. Thermal degradation of plastic has great interest as an alternative source of energy or value-added chemical, and it also contributes to fixing the challenges of environmental pollution. Here we studied thermogravimetric (TGA) techniques to obtain basic knowledge on degradation of low-density polyethylene (LDPE) over different acidic catalysts. The catalysts were characterized by XRD, NH3-TPD, BET and SEM. We studied hexadecane as a model compound. The hydrocracking of hexadecane was carried out in a batch reactor and the resultant products were analyzed by GC and GC-MS analysis.

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Poster Presentation : **MAT.P-404**

Material Chemistry

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Investigation of Photocatalytic Decomposition of Organic Dye in Wastewater Using Heterojunction Compounds of Ni-Doped CdS Nanoparticles and Fe_2O_3 Nanoparticles under Natural Light

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We synthesized Ni-doped CdS nanoparticles through a hydrothermal method and subsequently formed heterojunction nanocomposites with Fe_2O_3 nanoparticles, also prepared using the same approach. Our findings demonstrate that this heterocomplex exhibits superior efficiency compared to existing methodologies. Ni-doped CdS nanoparticles (Ni-CdS) were meticulously fabricated by controlling the amount of $Ni(AC)_2$, resulting in distinct variations denoted as Ni-CdS1, Ni-CdS2.5, Ni-CdS5, and Ni-CdS7.5. Notably, the most efficient heterojunction was observed between Ni-CdS5 and Fe_2O_3 nanoparticles, identified as Ni-CdS@Fe_2O_3. Characterization through scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction spectroscopy (XRD), and X-ray photoelectron spectroscopy (XPS) confirmed the presence of a well-defined heterojunction structure. The synthesized heterojunction nanocomposite exhibited remarkable efficacy in decomposing methylene blue (MB) solutions and proved to be a recyclable material. Ni-CdS@Fe_2O_3 displayed the highest photocatalytic activity, decomposing 97.33% of the MB solution under Xe lamp irradiation for 50 minutes. The photocatalytic decomposition performance of different types of dyes, rhodamine 6G (R6G), cargo red (CR), phenol, and bisphenol, was confirmed. Tests for reusability were also conducted three times, demonstrating higher effectiveness compared to existing studies. This enhanced photocatalytic efficiency is attributed to the unique properties created by the band gap reduction and abundance of active sites through the combination with magnetized Fe_2O_3.

Poster Presentation : **MAT.P-405**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Lead-Free Tin-Based Red and Green 2-D Perovskites

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Lead-Free Tin-Based Red and Green 2-D PerovskitesStephy Jose[1,2], Ji-Hoon Choi[1,2], Jae-Eun Pi[1],Joo Yeon Kim[1,2] 1. Reality Display Research Section, Reality Devices Research Division, ICT Creative Research Laboratory, Electronics and Telecommunications Research Institute, South Korea 2. Advanced Device Technology, ICT, University of Science and Technology, South Korea Corresponding Author: jooyeon.kim@etri.re.krAbstract: In general, metal halide perovskites (ABX_3forms) exhibit a high absorption coefficient, meaning they efficiently absorb light across a broad spectrum. One of the remarkable features is the tunability of their bandgap, allowing them to control the absorption and emission wavelength by adjusting the composition of the perovskites. Therefore, these materials have shown promise in various optoelectronic applications, including solar cells, light-emitting diodes (LEDs), photodetectors, and lasers.However, human safety and environmental regulation point of view, the toxicity of lead has to be a serious concern, which is strongly restricted to exploring industrial approaches. Therefore, as lead-free alternatives, tin-based perovskites have been suggested as a potential substitute because of their similar optoelectronic properties to lead-based perovskites. In this work, synthesized 2D tin-based halide perovskites, which are red and green emissive ones, are introduced to be applied as color conversion layers (CCL), and also their physical and optical properties were investigated. Key Words - lead-free, tin-based perovskite, color conversion layers AcknowledgmentThis work was partially supported by Electronics and Telecommunications Research Institute (ETRI) grant funded by the Korean

government [24ZC1200, Research on hyper-realistic interaction technology for five senses and emotional experience].This work was also partially by the Institute of Information & communications Technology Planning & Evaluation (IITP) grant funded by the Korea government(MSIT) [No.2022-0-00026, Near-eye light field device technology development for hyper-realistic metaverse service].This work was supported by the Technology Innovation Program Development Program-Development and Demonstration of New Market-creating Display Technology [20023880, Development and Demonstration of Space Hologram Based Non-contact Touch Input/Output Device] funded By the Ministry of Trade, Industry & Energy (MOTIE, Korea).

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Poster Presentation : **MAT.P-406**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

DNA-Guided Morphology Control of Plasmonic Metal Nanoparticles

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Here, we present two distinct DNA-based approaches for controlling the morphology and optical properties of plasmonic metal nanoparticles. First, we investigated metal overgrowth on gold nanoparticles modified with thiolated DNA, which showed varying morphologies depending on DNA sequences and ionic strengths. Second, we used area-selective functionalization of two different DNA sequences on gold nanoparticles for dynamically controllable site-specific self-assembly. Through this approach, we demonstrate DNA-induced morphological transitions between two different arrangements of nanosphere and ring structures. We anticipate that the dynamic structural tunability would allow for in-depth investigation of interparticle optical coupling in various geometries.

Poster Presentation : **MAT.P-407**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

Carbon-based Composite with ZnO and Ag_2O: Efficient Photocatalytic Decomposition of Hazardous Pollutants under Sunlight

Anil Pandey, Santu Shrestha, In Sup Lee, Narayan Gyawali, Subas Acharya, Vince Fualo, Siti Nur Syawalina Farahin, Jae Ryang Hahn*

Department of Chemistry, Jeonbuk National University, Korea

Efficient semiconductor photocatalysts face the significant challenge of electron recombination, limiting their performance in various applications. We proposed a promising approach to address this issue by combining multiwall carbon nanotubes (MWCNT) with semiconductor metal oxides. Herein, we synthesized a ternary composite of zinc oxide nanoparticles (ZONP), silver oxide nanoparticles (AONP), and MWCNT nanocomposite (abbreviated as ZAMC) through wet chemical, co-crystallization, and high-pressure annealing. Morphological investigations reveal that the MWCNT forms quick electronic conduction routes, connected by ZONP and AONP, creating a ternary heterojunction. The uniform distribution of ZONP, AONP, and MWCNT is confirmed through elemental analysis, further validating the development of the ternary heterojunction using comprehensive imaging and spectroscopic techniques. The as-synthesized ternary composite photocatalyst exhibits significantly enhanced photocatalytic activity compared to individual and binary composites. Notably, within 15 minutes of simulated sunlight exposure, the ZAMC sample demonstrates outstanding photocatalytic performance, achieving 96.06%, 92.03%, and 90.86% photo-deterioration of methylene blue, tetracycline, and ibuprofen solutions respectively. Furthermore, the ZAMC photocatalyst significantly improved bisphenol A decomposition, achieving 92.41% degradation in 50 min under simulated sunlight. After five cycles, the tests on reusability showed only a 7.74% decrease in performance. This improved photocatalytic performance is attributed to the synergistic migration of e−/h+ pairs along the conduction channels at the ZONP, AONP, and MWCNT interface, facilitating efficient charge separation and utilization.

Poster Presentation : **MAT.P-408**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

In situ confinement of copper/copper oxide nanoparticles inside a carbon tube using a single Cu-MOF precursor: a facile morphologically controlled synthesis strategy for superior oxygen evolution reaction and visible-light-driven photocatalytic efficiency

Narayan Gyawali, In Sup Lee, Santu Shrestha, Anil Pandey, Subas Acharya, Vince Fualo, Siti Nur Syawalina Farahin, Jae Ryang Hahn*

Department of Chemistry, Jeonbuk National University, Korea

A facile in situ process was developed to confine CuxO/Cu (x=1,2) particles (CUO) inside a carbon tube (CT) to produce composites (CUO-iCT) via a morphology-controlled synthesis of Cu-MOF-derived precursor that exhibits outstanding photocatalytic and oxygen evolution reaction (OER) efficiency. By modifying Cu-MOF as a single source, CUO could be trapped inside the CT, thereby overcoming two major barriers that have limited the overall catalytic efficacy of MOF-derived materials: aggregation/ agglomeration of CUO and improper alignment of the band structure. The confinement effect of the in situ developed carbon tube ensured the formation of a compact CUO-carbon heterojunction without clustering. The formation and confinement of CUO inside CT was confirmed with transmission electron microscopy (TEM), X-ray diffraction spectroscopy (XRD) and X-ray photoelectron spectroscopy (XPS). To test the applicability, CUO-iCT was used to catalyze the decomposition of cationic and anionic dyes under visible light (VL) and OER in an alkaline medium. The best-performing CUO-iCT resulted in the degradation of 98% of methylene blue in 80 min under VL, which is twice the efficacy of the standard commercial photocatalyst (TiO2). Moreover, the photocatalytic reaction showed a rate constant 17 times greater than the photolysis reaction. Similarly, the composite exhibited extraordinary OER activities in the alkaline medium, with a 283 mV overpotential and a Tafel slope of 58 mV/dec. The outstanding photocatalytic and electrocatalytic efficiency of CUO-iCT is attributed to unique morphology leading to a reduced bandgap, rich active sites, high surface-to-volume ratio, prolonged e--h+ separation, and confinement effect.

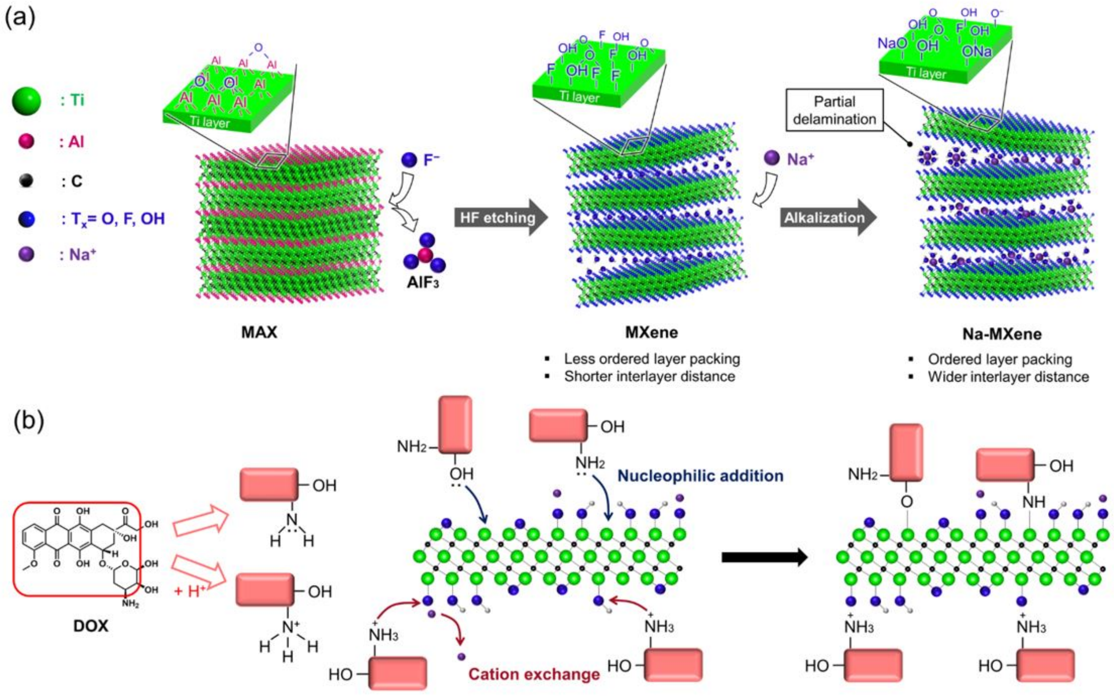
Poster Presentation : **MAT.P-409**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Selective adsorption of Doxorubicin via topotactic surface enrichment with hydrated Na^2 ions on engineered MXene nanosheets

Zubair Khalid, Jae-Min Oh[1,*]

Energy and Materials, Dongguk University, Korea
[1] *Department of Energy and Materials Engineering, Dongguk University, Korea*

Effective adsorption (250 mg/g) of water-soluble drug, doxorubicin, was achieved by utilizing a surface functionalized two-dimensional transition metal carbide (MXene) in an alkaline solution. The powder X-ray diffraction (XRD) patterns suggested the alkalized MXene (Na-MXene) had higher crystallinity than the MXene regardless of the higher surface area. Scanning electron microscopic (SEM) images revealed thicker layers in the particle of a Na-MXene than that of the MXene, which accompanied partial delamination. X-ray photoelectron spectroscopy (XPS) indicated the O-rich surface of Na-MXene to show better interlayer packing compared to the MXene. Doxorubicin was adsorbed on Na-MXene with pseudo-second-order kinetics with single layer. A XPS spectrum after adsorption suggested that doxorubicin adsorbed by cation exchange and nucleophilic addition. The strong affinity of the primary amino group to the MXene layer allowed selective adsorption of doxorubicin compared to dyes with secondary, tertiary and aniline like amino groups.


(a)
: Ti
: Al
: C
: T_x= O, F, OH
: Na^+
Ti layer
F^-
AlF_3
HF etching
MAX
MXene
Less ordered layer packing
Shorter interlayer distance
Na^+
Alkalization
Partial delamination
Na-MXene
Ordered layer packing
Wider interlayer distance
(b)
DOX
+ H^+
Nucleophilic addition
Cation exchange
NH_2
OH
NH_3
HO
NH
O

Poster Presentation : **MAT.P-410**

Material Chemistry

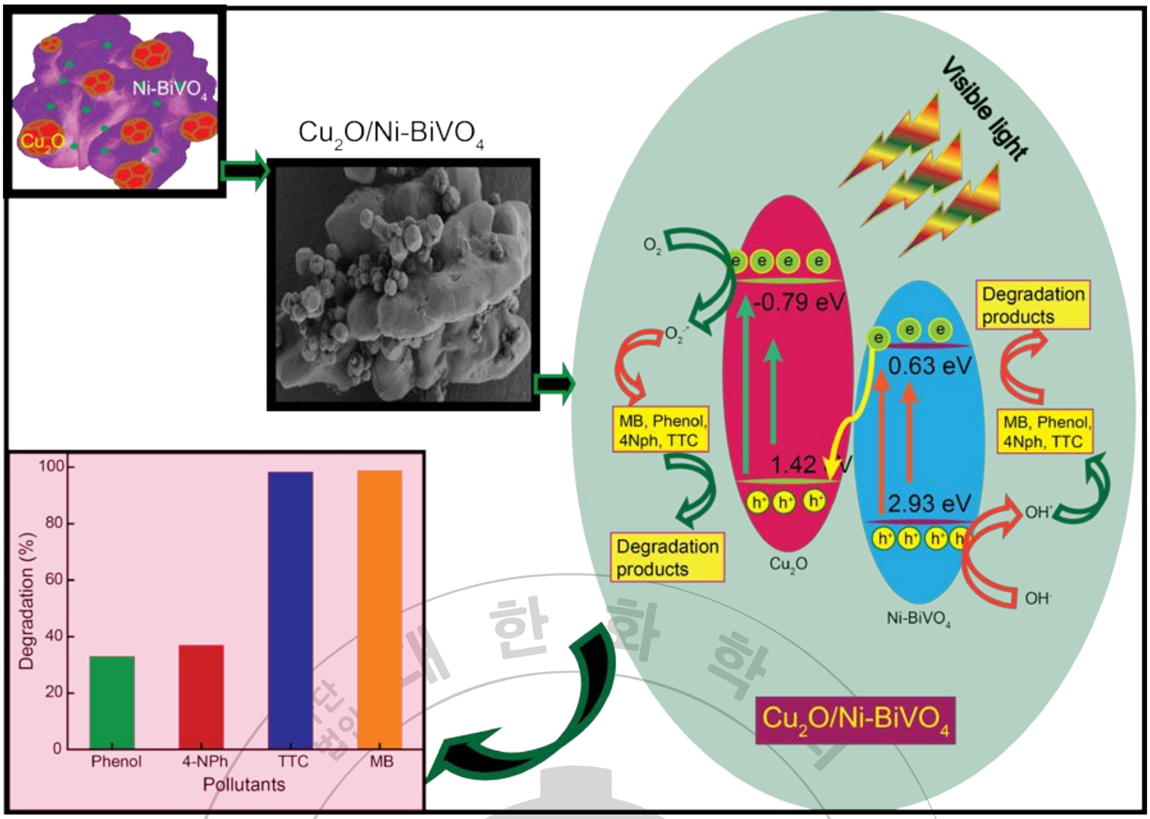
Exhibition Hall 2 THU 11:00~13:00

Ni doping and Cu_2O decoration on $BiVO_4$ for bandgap tuning and application to pollutant degradation under visible light

Santu Shrestha, Narayan Gyawali, In Sup Lee, Anil Pandey, Subas Acharya, Vince Fualo, Siti Nur Syawalina Farahin, Jae Ryang Hahn*

Department of Chemistry, Jeonbuk National University, Korea

The extensive use, continuous-release, and persistent existence of organic pollutants have caused serious damage to the aquatic environment and human health, thereby necessitating an eco-friendly and efficient remediation of these contaminants. In this context, we synthesized Ni-doped $BiVO_4$ (Ni-BVO) and Cu_2O/Ni-$BiVO_4$ (CNBVO) composites by doping Ni onto bismuth vanadate (BVO) and decorating truncated octahedral Cu_2O nanoparticles onto the Ni-BVO via a modified hydrothermal method to achieve extended visible-light absorption, bandgap tuning, and effective separation of charged species. The synthesized composites were tested for photocatalytic decomposition of several pollutants, including phenol, 4-nitrophenol, tetracycline, and methylene blue molecules, to demonstrate their broad applicability. The CNBVO photocatalyst exhibited complete degradation (~98.8%) of methylene blue and tetracycline (98.2%) within 110 min. The photodegradation followed a first-order reaction with CNBVO, whose rate constant is 308%, 176%, and 161% of the rate constants of bare Cu_2O, BVO, and Ni-BVO, respectively. CNBVO showed robust stability for three subsequent cycles and is an efficient and promising composite catalyst for environmental remediation.


Ni-BiVO$_4$
Cu$_2$O
Cu$_2$O/Ni-BiVO$_4$
Visible light
O$_2$
O$_2^{\cdot-}$
e e e e
-0.79 eV
e e e
0.63 eV
1.42 eV
2.93 eV
h$^+$ h$^+$ h$^+$
h$^+$ h$^+$ h$^+$ h$^+$
Cu$_2$O
Ni-BiVO$_4$
MB, Phenol, 4Nph, TTC
Degradation products
MB, Phenol, 4Nph, TTC
Degradation products
OH$^{\cdot}$
OH$^-$
Cu$_2$O/Ni-BiVO$_4$
Degradation (%)
0
20
40
60
80
100
Phenol
4-NPh
TTC
MB
Pollutants

Poster Presentation : **MAT.P-411**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Investigation of the CO_2 Absorption Ability of A_2CO_3-promoted CdO(A=Li, Na and K) in Intermediate Temperature Range

Kang-Yeong Kim, **Young-Uk Kwon**[1,*]

CO2 Utilization Research Center, Korea Institute of Geoscience and Mineral Resources, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

In this study, we investigated the CO_2 absorption ability of A_2CO_3-promoted CdO (A=Li, Na and K) in the intermediate temperature range (270–400 °C). While CdO mixed with Li_2CO_3 does not absorb CO_2 at 270–330 °C, but Na_2CO_3- and K_2CO_3- promoted CdO react with CO_2 at 270–320 °C and 270–390 °C, respectively. Each product of CO_2 absorption was confirmed to the double carbonate containing Na and Cd and K and Cd of which crystal structures are analogous to fairchildite($P6_3/mmc$, $K_2Ca(CO_3)_2$) and nyerereite($P6_3mc$, $Na_{1.67}K_{0.33}Ca(CO_3)_2$), respectively. Both show repetitive CO_2 absorption ability in cycling test in which absorption and desorption are continually alternated. In addition, These Na_2CO_3- and K_2CO_3-promoted CdO can react with CO_2 under 50 vol% CO_2.

Poster Presentation : **MAT.P-412**

Material Chemistry

Exhibition Hall 2 THU 11:00~13:00

DNA-Linked Nanoparticle Films for Shape Morphing by Light Stimulation

Seonju Park, Jong Wook Kim[1], So-Jung Park[2,*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

[1]*Ewha Womans University, Korea*

[2]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*

Soft actuators that respond to specific stimuli have potential in various fields, including biomedicine, as they can implement the unique advantages of living organisms, such as flexibility, adaptability, and reorganization. Among various stimuli, light has a great advantage in the area of precision. Here, we fabricated a free-standing nanoparticle film using light-activatable hairpin DNA as a light-responsive soft actuator. This approach involves the construction of multicomponent plasmonic nanoparticle films by DNA-directed bottom-up layer-by-layer (LbL) self-assembly followed by top-down photopatterning using the photothermal property of metal nanoparticles. The hairpin DNA in the nanoparticle film can be opened by light illumination through the photothermal effect of metal nanoparticles, which can cause morphological changes of the film. The presentation will discuss structure-dependent light responsivity and design principles for effective light-induced structural control.

Poster Presentation : **MAT.P-413**
Material Chemistry
Exhibition Hall 2 THU 11:00~13:00

Quantum Dot Composite Colloids with Layer-by-Layer Shell and Their Biological Self-assemblies for Signal Amplified Detection

Bomi Kim, Sung Jee Kim*

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

The quantum dot composite colloid (QDCC) can be defined as tens of nanometer to micron-sized colloidal particles that contain multiple QDs. Herein, we report polyelectrolyte shell decorated QDCCs, which were decorated by cationic (polyethylenimine, PEI)/anionic (poly(sodium 4-styrene sulfonate), PSS) polyelectrolytes in a Layer-by-Layer (LbL) method over cores of amphiphilic PEI-derivative composites (QD-amPEI). Structural plasticity and colloidal stability of QDCCs could be obtained by tuning the LbL shells of QDCCs, which include ions permeation of QDCC shell, fusion/fission of QDCCs accompanying partial exchange between the payloads, and enhanced colloidal stabilities in a broad pH range and high salt concentrations. The outer layer of QDCC shells was decorated by amines, carboxylates, zwitterionic moieties, or a combination of those, which endowed QDCCs with flexible bioconjugation capability and low non-specific adsorption level. As a proof-of-concept, signal amplification for C-reactive protein (CRP) was demonstrated using biotin-avidin motif-assisted biological self-assembly of QDCCs. The signal amplification was applied to FL immunoassay platform, where rapid (~ 6 minutes) and sub-picomolar sensitive detection was successfully achieved.

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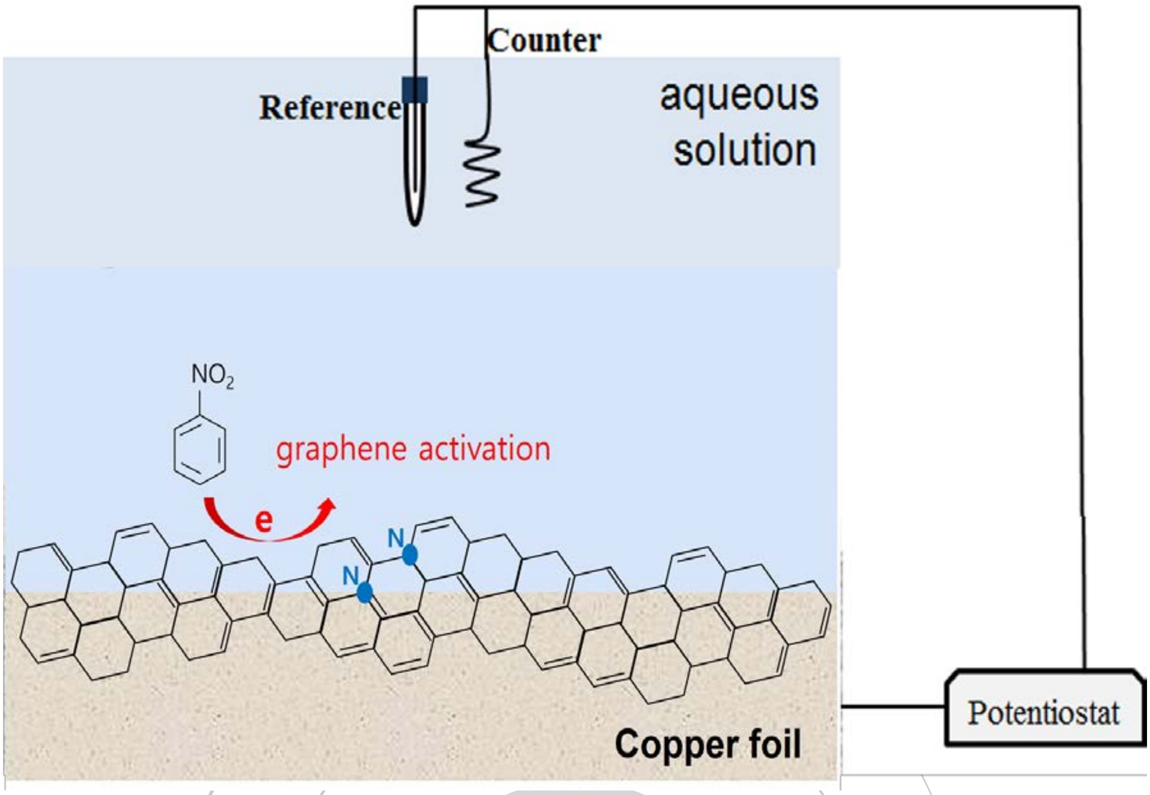
Poster Presentation : **ELEC.P-395**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Electrochemical Activation of Graphene coated on the copper electrode by Nitrobenzene Reduction

Jin-Young Lee[*], **Dong Jin Kim**[1]

Department of Chemical Engineering and Biotechnology, Tech University of Korea, Korea
[1]*Chemoinformatics Research, Korea Institute of Science and Technology, Korea*

The Cu electrode was covered with chemical vapor deposition (CVD) graphene and used as for an electrochemical reduction reaction of nitrobenzene (NB) in the aqueous solution. After NB reduction at -0.6 V (vs. Ag/AgCl) for 10 min, the charge transfer impedance for NB reduction decreases. As NB gets reduced, CVD graphene-covered Cu electrode is electrochemically activated.On the activated graphene-coated copper by NB reduction, nitrogen atom was observed by XPS (X-ray Photoelectron Spectroscopy). It suggests that NB reduction causes graphene-coated copper electrode to activates such as N-doped graphene.


Counter
Reference
aqueous solution
NO_2
graphene activation
e
N
N
Copper foil
Potentiostat

Poster Presentation : **ELEC.P-396**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Advancing Electrochemical Impedance Spectroscopy: Integrating Deep Learning for Enhanced Analysis and Precision

Byoung-Yong Chang

Department of Chemistry, Pukyong National University, Korea

Recent advancements in Electrochemical Impedance Spectroscopy (EIS) have facilitated the rapid acquisition of extensive spectral datasets within shorter timeframes. However, traditional analysis methods have found it challenging to match the pace of these technological innovations. To address this gap, our study introduces a groundbreaking approach that harnesses the power of deep learning for evaluating electrochemical impedance spectra under varying potentials. At the heart of this method is the use of an auto-encoder, a specialized type of deep neural network. This auto-encoder efficiently converts impedance data into two-dimensional latent vectors, effectively capturing the essence of electrochemical reactions related to shifts in electrode potential. These vectors represent fundamental phenomena such as charge transfer, mass transfer, and electric double-layer charging. Upon decoding, these latent vectors provide impedance spectra with enhanced clarity and precision. Our findings present a strong proof of concept, underscoring the potential of integrating machine learning to automate and refine EIS analysis

Poster Presentation : **ELEC.P-397**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Design of glycol gel electrolytes for supercapacitors operable at extreme temperatures

Nagyeong Jeon, 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*

Gel electrolytes for supercapacitors require excellent mechanical properties and high ionic conductivity. Hydrogel, commonly used as a gel electrolyte, has the limitation that it can only be used at temperatures between 0~100 ℃ because it is based on a water solvent. This study used a glycol solvent with a freezing point of -13 ℃ and a boiling point of 197 ℃ to create a robust glycol gel electrolyte. Additionally, the surface of the gel electrolyte was optimized to improve the adhesion of the gel, increasing compatibility and reducing resistance at the electrode interface. As a result, the electrochemical properties CV and GCD show consistent electrochemical behavior at extremely low and extremely high temperatures. This presentation describes the design of a glycol gel electrolyte with toughness, excellent electrode adhesion, and its performance as a supercapacitor operating over a wide range of temperatures.

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Poster Presentation : **ELEC.P-398**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Surface defect-induced OER and HER in Ru-doped metal-organic framework

Boka Fikadu Banti, Jaebeom Lee[1,*]

Department of Chemistry, Chungnam National University, Ethiopia

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

Surface defect-induced OER and HER in Ru-doped metal-organic framework Boka Fikadu Banti1, Jaebeom Lee1*1 Department of Chemistry Chungnam National University, Daejeon, 34134, Republic of KoreaCorresponding author: Jaebeom Lee, nanoleelab@cnu.ac.krAbstractThe Metal-organic frameworks (MOFs) are at the forefront of electrocatalysts for the HER, OER, and overall water splitting, due to their large surface area, numerous sites of activity, and appropriate pore sizes. Herein, we present a facile strategy for surface engineering of Ru-doped MOFs for efficient bifunctional catalysts for both H2 and O2 generation. A defective engineered surface for enhanced electrochemical reaction was achieved through selective etching of the polyhedron MOF that lead to transformation into a cubic morphology. The surface-engineered Ru-doped MOF/MoS2 heterointerface showed enhanced performance with a lower overpotential of 360 mV, and an enhanced current density of 87.9 mV dec-1 for both HER and OER when compared to the catalytic activities of individual Co-ZIF and Ru-doped Co-ZIF polyhedrons. Predictably, the Ru-Co-ZIF@MoS2 reveals greater OER and HER activity and stability in comparison to several bifunctional catalysts that have been reported, hence emphasizing its promise as a modern bifunctional electrocatalyst.Keywords: Catalysts, Bifunctional, MOF, Heterostructures, Ru-doped, and overpotential.

Poster Presentation : **ELEC.P-399**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

High Energy Density Single-Crystal NMC/Li6PS5Cl/ Ga-Li7La3Zr2O12 Cathodes for All-Solid-State Lithium-Metal Batteries

Sungwon Hwang

Department of System Semiconductor Engineering, Sangmyung University, Korea

Solid-state batteries replace commercial lithium-ion batteries due to their high energy density and safety. To achieve the high capacity of metal anodes, all-solid-state batteries require high energy density and long-lasting composite anodes, such as Ni-Mn-Co (NMC)-based lithium oxide mixed with hybrid solid electrolyte (SSE). However, in practice, the cathode capacity typically decreases due to increased NMC/SSE interface defects due to NMC cracking and NMC pulverization, which is only partially alleviated by applying high cell pressure during cycling. Using a low-temperature dry protocol, we report single-crystal particulate LiNi0.83Mn0.06Co0.11O2 and Li6PS5Cl /Ga-Li7La3Zr2O12 hybrid SSE composite cathodes with an outstanding discharge capacity of 220 mA h g−1 at 30 °C. Despite a 4.9% volume change during charge/discharge cycling, a first cycle coulombic efficiency of >88 and >99% thereafter was achieved. A nearly realistic high-steady discharge capacity at a high areal capacity of 9.5 mA·h cm-2 was obtained using asymmetric anode/cathode cycling pressures of only 2.0 MPa/0.5 MPa. After adding LLZO to the LPSCl electrolyte, the cycling stability of the hybrid solid electrolyte and its performance for all-solid-state batteries were significantly improved. Therefore, the single crystal particulate LiNi0.83Mn0.06Co0.11O2 and Li6PS5Cl /Ga-Li7La3Zr2O12 hybrid composite structure is a promising structure for high-performance all-solid-state batteries for electric vehicles.

Poster Presentation : **ELEC.P-400**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Harnessing the Electro-Inductive Effect for Tunable Emission Wavelengths in Iridium Cyclometalated Complexes

Seunghwan Eom, Eunji Lee, Mu-Hyun Baik*

Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Korea

The Electron-Inductive Effect (EIE)[1] has demonstrated the ability of the electrode to replace the functional group and modify the molecule's properties. To change the emission wavelength of the emitter molecule, maximizing the electro-inductive effect involves separating its frontier orbitals. By positioning the HOMO closer to the electrode than the LUMO, applying a positive voltage results in a significant decrease in HOMO energy relative to LUMO energy.

The $[Ir(ppy)_2(bpy)]PF_6$ cyclometalated complexes, composed of iridium(phenylpyridine)$_2$(bipyridine), are employed as the target system for investigating the effect of the electro-inductive effect on wavelength changes. These complexes exhibit diverse emission colors based on the different functionalizations of the ppy and bpy ligands, which have been extensively studied.[2] To facilitate this, thioacetate-functionalized Ir complexes ($[Ir(SAc\text{–}ppy^{3,4})_2(bpy)]PF_6$) were synthesized to form a self-assembled monolayer via ppy side on a gold substrate.[5]

Reference

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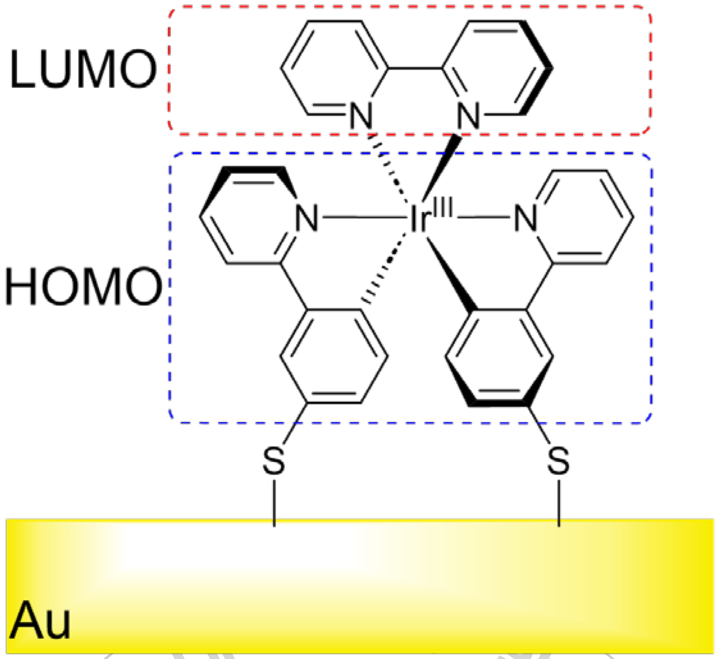
LUMO
HOMO
N
N
N
Ir^{III}
N
S
S
Au

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Poster Presentation : **ELEC.P-401**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Perturbation of Na-ion distribution for enhancement of ionic conductivity to a practical level of over 1 mS·cm^{-1} in Na_3ZnGaS_4

Jungyong Seo, Myoungho Pyo*

Department of Advanced Components and Materials Engineering, Suncheon National University, Korea

Na-ion conducting solid-state electrolytes (SSEs) are increasingly drawing an attention as a potential alternative to Li-ion conducting SSEs in all-solid-state batteries. In this work, we describe the replacement of a small fraction of S^{2-} by I^- causes a perturbation of Na-ion distributions, which increases a vacancy concentration in already known Na conduction channels (Na2 sites) and generates a new conduction route (Na3 sites). As a result of dual contributions by I-substitution, the ionic conductivity (σ_{ion}) of $Na_{3-x}ZnGaS_{4-x}I_x$ remarkably increases from ~10^{-3} mS cm^{-1} in pristine Na_3ZnGaS_4 to > 1 mS cm^{-1} in $Na_{2.9}ZnGaS_{3.9}I_{0.1}$, which cannot be attained by a stoichiometric vacancy incorporation alone. Incorporation of less (x = 0.05) or more (x = 0.15 and 0.2) amounts of I^- also results in a significant improvement of σ_{ion}, revealing the effectiveness of Na-site disturbance. Cl- or Br-doped Na_3ZnGaS_4 also shows the improvement of σ_{ion}, but a degree of improvement is limited. The presence of iodides in a specific sulfur site (S3 site) and Na-dispersion between Na2/Na3 sites are validated via theoretical, crystallographic, and spectroscopic studies. The electrochemical and moisture stability of $Na_{2.9}ZnGaS_{3.9}I_{0.1}$ is also demonstrated. Finally, benefiting from the electrochemical stability and high σ_{ion}, the practicality of $Na_{2.9}ZnGaS_{3.9}I_{0.1}$ in all-solid-state batteries is exemplified using $Na_2Sn \parallel TiS_2$ full cells.

Poster Presentation : **ELEC.P-402**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Electrochemical DNA Cleavage Sensing for EcoRV with an ERGO Electrode

Hyunbeom Kim, Tae Hyun Kim[1,*]

Chemistry, Soonchunhyang University, Korea

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

Herein, we present a novel electrochemical assay for EcoRV activity using electrochemically reduced graphene oxide (ERGO). EcoRV belongs to the type II restriction endonuclease family, enzymes that hydrolyze the internal phosphodiester bonds in deoxyribonucleic acid (DNA) or ribonucleic acid (RNA). Specifically, EcoRV can cleave duplex DNA at the TA site of the target sequence GATATC.In our study, we employed the electrochemical assay based on MB-DNA/ERGO-GCE (glassy carbon electrode) for the detection of EcoRV. The choice of ERGO was driven by its eco-friendliness, high efficiency, energy-saving properties, and controllability. Methylene blue (MB) tagged double-stranded (ds) DNA, featuring a single-stranded (ss) segment at the end for anchoring on graphene through π-π stacking, was utilized for the detection of EcoRV. The electrochemical current signal was reduced after EcoRV cleaved the dsDNA-MB.The assay demonstrated excellent specificity and high sensitivity, with a limit of detection (LOD) of 9.5 × 10−3 U mL−1. Notably, the assay could be conducted in the presence or absence of acrintricarboxylic acid, functioning as an EcoRV inhibitor.

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Poster Presentation : **ELEC.P-403**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Metal-Organic Framework-Derived Co3O4/NiCo2O4 DSNCs as an Electrochemical Sensor for the detection of Alfuzosin

Amin Al, Tae Hyun Kim[1,*]

Chemistry, Soonchunhyang University, Korea

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

This study presents the development of Co3O4/NiCo2O4 double-shelled nanocomposites (DSNCs) as an electrochemical sensor for the sensitive and selective detection of alfuzosin, a medication used for benign prostatic hyperplasia (BPH). The DSNCs were synthesized using a metal-organic framework (MOF) route, offering precise control over morphology and composition. Physicochemical characterization techniques like X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), field emission scanning electron microscopy (FE-SEM), and high-resolution transmission electron microscopy (HR-TEM) confirmed the successful synthesis and structural features of the DSNCs. Electrochemical analysis employing cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques demonstrated the efficient electrocatalytic activity of the DSNCs towards alfuzosin. The sensor, fabricated by modifying a glassy carbon electrode (GCE) with the DSNCs, exhibited an impressive linear detection range of 5–180 μM and a remarkably low limit of detection (LOD) of 1.366 μM. Furthermore, the sensor displayed excellent selectivity for alfuzosin, along with outstanding reproducibility and long-term stability. The applicability of the sensor was validated through real sample analysis of alfuzosin in pharmaceutical tablets and human serum, achieving satisfactory recovery rates. These findings highlight the Co3O4/NiCo2O4 DSNCs as a promising candidate for the development of a highly sensitive, selective, and robust electrochemical sensor for alfuzosin detection, holding immense potential in therapeutic drug monitoring, clinical diagnostics, and environmental monitoring applications.

Poster Presentation : **ELEC.P-404**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Acid-base dual doped graphene for electrochemical urea synthesis.

Sungtae Kim, Jun Hyeok Kwon, Tae-Hyuk Kwon[*]

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

Artificial nitrogen fixation has played a pivotal role in sustaining population growth, with the Haber process being instrumental in producing ammonia from nitrogen and hydrogen gas. One of its primary applications is the production of urea, utilizing carbon dioxide. However, both ammonia synthesis and urea production require harsh conditions (high temperature, high pressure) and significant energy consumption. In this study, we present a novel approach to urea synthesis directly from CO2 and N2 using an acid-base co-doped graphene catalyst. By employing sonocavitation and nebulization synthesis (SNS), we create high-pressure, high-temperature reaction conditions via acoustic cavitation. Through the SNS method, we synthesize acid-base co-doped graphene, where acid and base sites interact with carbon dioxide and nitrogen. The acid component binds the reactants (CO2, N2), while the base site reduces the activation energy during the reduction process. Additionally, the hydrophobic graphene skeleton suppresses the hydrogen evolution reaction (HER), resulting in high faradaic efficiency for urea synthesis. To further enhance urea production, we focus on improving the current density of the catalyst. Utilizing a layer-by-layer (LBL) structure, we aim to enhance electrochemical properties and increase the three-phase (gas, liquid, and solid) surface area. Consequently, we propose that our catalyst offers a sustainable approach to green urea synthesis.

Poster Presentation : **ELEC.P-405**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Evidence of Intrinsic Pseudocapacitive Lithium Intercalation in Rutile $TiNbO_4$

Woowon Chung, Jin Ho Bang[1,*]

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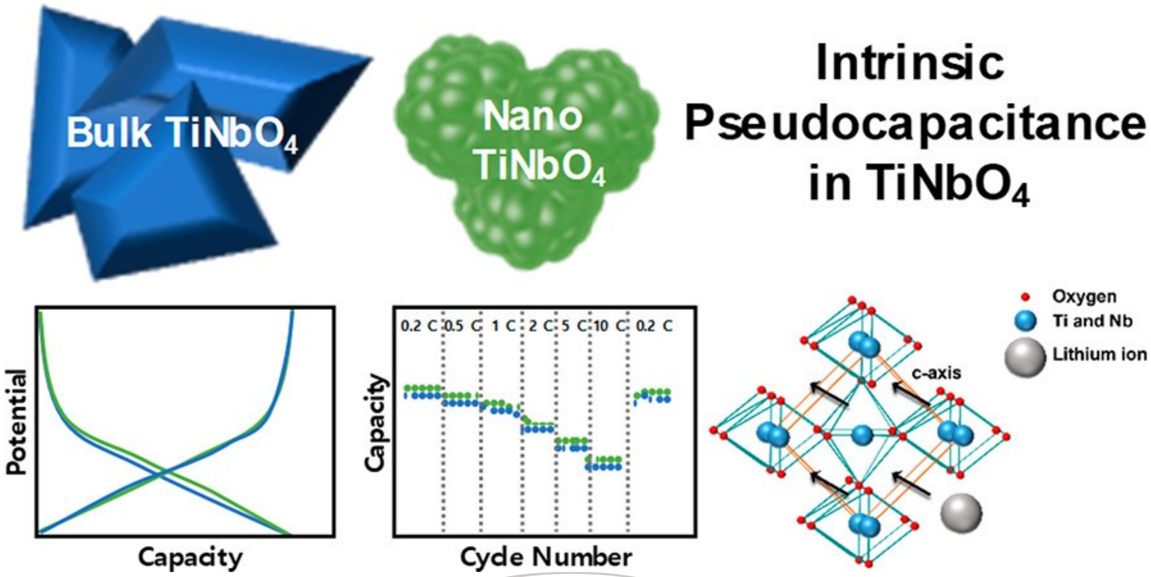
[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*

Entropy-stabilized titanium niobium oxides (TNOs) with crystallographic shear structures (e.g., $TiNb_2O_7$ and $Ti_2Nb_{10}O_{29}$) are generally synthesized by high-temperature calcination in an air or an oxygen atmosphere to compensate for their positive enthalpies of formation. In previous paper, we demonstrate that changing the reaction atmosphere into a slightly reductive environment using in situ carbonization leads to the creation of a new class of TNO with a formula of $TiNbO_4$. Unlike its predecessors, this new lithium reservoir is a rutile phase, and most strikingly, in situ X-ray diffraction analysis revealed that its lithium intercalation occurs via a purely solid-solution process. Since solid-electrolyte-interface-free, high capacity anode materials with long cyclic life are required to meet the stringent requirements of widespread lithium-ion battery utilization, this finding of a new electrode material with purely single-phase lithium intercalation is of great interest for the development of high-performance anode materials. Distinctive electrochemical behavior that is different from that of crystallographic shear structured TNO is revealed by in-depth electrochemical analyses, which is ascribed to the unique structural and electronic properties of $TiNbO_4$. In this work, we show that $TiNbO_4$ stores Li-ions via intercalation pseudocapacitance in both bulk and nanostructured states. The rate performance and capacity of $TiNbO_4$ are independent of nanostructuring, indicating that $TiNbO_4$ stores charges through an intrinsic pseudocapacitance mechanism.


Bulk TiNbO4
Nano TiNbO4
Intrinsic Pseudocapacitance in TiNbO4
Potential
Capacity
0.2 C
0.5 C
1 C
2 C
5 C
10 C
0.2 C
Capacity
Cycle Number
Oxygen
Ti and Nb
Lithium ion
c-axis

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Poster Presentation : **ELEC.P-406**
Electrochemistry
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Theoretical Studies on the (ReV)X_2 (X = S, Se) Alloy Nanosheets as Hydrogen Evolution Reaction Electrocatalysts

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[1] *Department of Materials Chemistry, Korea University, Korea*
[2] *Department of Nano & Advanced Materials Engineerin, Jeonju University, Korea*

It is challenging to control the electronic structure of two-dimensional transition metal dichalcogenides (TMD) for extended applications in renewable energy devices. In this study, we performed first-principles calculations on (ReV)X_2 (= $ReSe_2$-VSe_2 and ReS_2-VS_2) alloy nanosheets. Increasing V composition makes the nanosheets more metallic and induces a 1T″-to-1T phase transition. Compared to the $MoSe_2$-VSe_2 and WSe_2-VSe_2 alloy nanosheets, Re and V atoms were mixed more homogeneously at the atomic scale. Density of states and Gibbs free energy calculations showed that alloying increased the metallicity and thus effectively activated the metal or chalcogen atoms toward the HER, supporting the observed increased HER performance of the alloy nanosheets. Fermi abundance function, and Bader charge further supports that the alloying enhances the catalytic HER activity of nanosheets. Our study provides a strategy for designing new TMD alloy nanosheets with enhanced catalytic activity.

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Poster Presentation : **ELEC.P-407**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Chiral catalyst effect of twisted nanowire bundles for photoelectrochemical water splitting

Goddati Mahendra, **Jaebeom Lee**[1,*]

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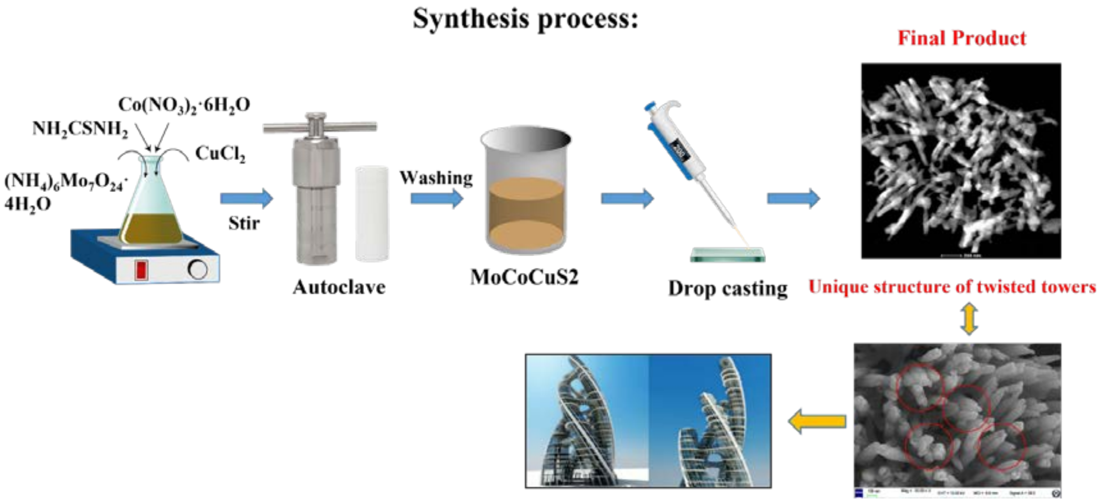
[1]*Chemistry, Chungnam National University, Korea*

The overexploitation of fossil fuels has made developing alternative energy sources an essential priority for many decades. The photoelectrochemical (PEC) splitting of water is a potential technique for hydrogen generation, which is considered the fuel of the future owing to the high enthalpy of combustion. PEC water splitting efficiency still needs to be improved from volume hydrogen production and requires additional efforts. Recently, it has been shown that chirality is essential in resolving problems associated with PEC water splitting by the effects of chiral-induced spin control and chiral-enhanced light harvesting. When it comes to increasing the effectiveness of water splitting, it is about time that attention was paid to the art of chirality. Methods for introducing chirality structure into photocatalysts for PEC water splitting are characterized using the techniques applied in this research work. The present study proposes an innovative approach to induce a chiral effect using a unique nanostructure, i.e., twisted nanowire bundle structures, which can obtain additional light. The utilization of computational modelling provides evidence for the inherited catalytic characteristics and facilitates the observation of the optimum geometric configuration of nanowires. The challenges of activating PEC water splitting are discussed, and its bright future is anticipated.


Synthesis process:
Final Product
$Co(NO_3)_2 \cdot 6H_2O$
NH_2CSNH_2
$CuCl_2$
$(NH_4)_6Mo_7O_{24} \cdot 4H_2O$
Stir
Autoclave
Washing
MoCoCuS2
Drop casting
Unique structure of twisted towers

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Poster Presentation : **ELEC.P-408**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Computational Insights into the Electron-Inductive Effect using FC-DFT: Linker Effects and Potential Window Enhancement

Kyujun Lee

Chemistry, Korea Advanced Institute of Science and Technology, Korea

By applying voltage, the ability to adjust the properties of molecules immobilized on electrodes has been previously reported. Subsequently, the vibrational Stark shift in the Raman spectrum of immobilized molecules was detected. Fractional Charge-Density Functional Theory (FC-DFT) can provide consistent calculations for this experimental tuning rate. However, a limitation of prior research is the minimal Electro-inductive effect (EIE) due to an insufficient potential window. This study investigates the effects resulting from the differences in linkers connecting the gold surface and immobilized molecules, analyzing their impact. Strategies are explored to widen the potential window, aiming to enhance the efficiency of the EIE. Furthermore, computational explanations are provided using FC-DFT.

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Poster Presentation : **ELEC.P-409**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Suppressing hydrogen evolution in N_2 reduction by heteroatom doped graphene.

Jun Hyeok Kwon, Sungtae Kim, Tae-Hyuk Kwon*

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

Ammonia (NH_3) is one of the most significant chemicals because it plays a vital role in the chemical and hydrogen storage industry. The most of ammonia was synthesized by Haber-Bosch process. However, Haber-Bosch process consumes enormous energy and emits green house gasses. Therefore, a sustainable and eco-friendly method is highly required. Electrochemical nitrogen reduction reaction (eNRR) emerges as an alternative method that make ammonia at ambient conditions. However, eNRR is still difficult to commercialize because of its low NRR Faradaic efficiency (FE). The main reason of low NRR FE is a competitive hydrogen evolution reaction (HER). HER is kinetically more favorable than NRR. Therefore, HER suppression is key point to increase NRR performance. Herein, we introduced heteroatom doped graphene layer for suppressing a hydrogen evolution reaction (HER) to improve a nitrogen reduction reaction (NRR). A hydrophobicity of graphene could restrict accessibility of hydrogen source of water. Furthermore, heteroatoms doped in graphene could change electrical properties of graphene. As a result, heteroatom doped graphene was able to suppress HER by effectively restricting the hydrogen sources.

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Poster Presentation : **ELEC.P-410**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Imaging Single Nanobubbles of H_2 during Water Splitting using In-Situ Electrochemical-Fluorescence Lifetime Imaging

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Department of Chemistry, The Catholic University of Korea, Korea

[1]*Graduate School of Analytical Science and Technology (GRAST), Chungnam National University, Korea*

We describe the use of time-resolved fluorescence lifetime to image transient formation of single nanobubbles at the electrode/solution interface during electrocatalytic water splitting. The formation of single hydrogen nanobubbles was imaged in real time during a potential scan using in-situ electrochemical-fluorescence lifetime imaging (EC-FLIM). Hydrogen nanobubbles are generated from the reduction of water on the surface of Ni-Mo-based electrocatalysts modified FTO electrode and fluorescently imaged from the transient adsorption process of sulforhodamine G (SRG) molecules at the nanobubble surface. The ability to label and fluorescently image individual nanobubbles with SRG suggests that the gas/solution interface is hydrophobic in nature. From the intriguing observations, this method can serve as an analytical tool to image single nanobubbles on an electrode surface enabled us to observe in real time process during electrochemical gas generation.

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Poster Presentation : **ELEC.P-411**
Electrochemistry
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Temperature-Dependent Effect of Mn Substitution on $LiNiO_2$

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[1] *Department of Chemical & Molecular Engineering, Hanyang University, Korea*

Despite the important role of manganese (Mn) in cobalt-free, Ni-rich cathode materials, existing reports on the effects of Mn as a substitute for cobalt are not consistent. In this work, we analyzed the performance of cathodes comprised of $Li(Ni_{1-x}Mn_x)O_2$ (LNMO). Both beneficial and detrimental results occurred as a result of the Mn substitution. We found that a complex interplay of effects (Li/Ni mixing driven by magnetic frustration, grain growth suppression, and retarded lithium insertion/extraction kinetics) influenced the performance and was intimately related to calcination temperature. This indicates the importance of establishing an optimal reaction temperature for the development of high-performance LNMO.

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Poster Presentation : **ELEC.P-412**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Promoting Photocurrent in Au-TiO2 Electrodes via Cooperative Hole Scavenging

Mohsin Ali, Jin Ho Bang[1,*]

Applied Chemistry, Hanyang University, Korea
[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*

Recently, gold nanoclusters (Au NCs) have garnered significant attention as promising photosensitizers for TiO2-based photoelectrodes. However, a clear understanding of the underlying mechanisms occurring at the photoelectrode-electrolyte interface remains elusive. Beyond the size of Au NCs, the electrolyte composition critically influences the hole transfer mechanism. Notably, incorporating the less efficient hole scavenger ethylenediaminetetraacetic acid (EDTA) alongside sodium sulfite (Na2SO3), a stronger scavenger, impacts the photoelectrode’s catalytic activity. In this system, EDTA functions as a mediator, facilitating efficient hole/charge transfer in conjunction with Na2SO3. Our work unveils a remarkable phenomenon: the hole transfer mechanism is dictated by the driving force generated by varying Au NC sizes. This distinct behavior is elucidated through J-V curves and photoelectrochemical impedance spectroscopy.

Recently, gold nanoclusters (Au NCs) have garnered significant attention as promising photosensitizers for TiO_2-based photoelectrodes. However, a clear understanding of the underlying mechanisms occurring at the photoelectrode-electrolyte interface remains elusive. Beyond the size of Au NCs, the electrolyte composition critically influences the hole transfer mechanism. Notably, incorporating the less efficient hole scavenger ethylenediaminetetraacetic acid (EDTA) alongside sodium sulfite (Na_2SO_3), a stronger scavenger, impacts the photoelectrode's catalytic activity. In this system, EDTA functions as a mediator, facilitating efficient hole/charge transfer in conjunction with Na_2SO_3. Our work unveils a remarkable phenomenon: the hole transfer mechanism is dictated by the driving force generated by varying Au NC sizes. This distinct behavior is elucidated through J-V curves and photoelectrochemical impedance spectroscopy.

Poster Presentation : **ELEC.P-413**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Exploring TiNbO4 as a Promising Alternative to Li4Ti5O12

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Applied Chemistry, Hanyang University Erica, Korea

[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*

Driven by the ever-increasing demand and usage of lithium-ion batteries, researchers are continuously striving to advance their performance. While all major components play a crucial role, the anode material’s properties are paramount in determining the overall electrochemical performance of a battery cell. In this regard, Li4Ti5O12 has been favored over graphite due to its minimal volumetric changes. However, it suffers from significant drawbacks such as degassing, low electrical conductivity, and limited specific capacity. This study proposes TiNbO4 as a promising candidate to address these challenges. Operating between a 0-3V potential window, TiNbO4 exhibits a remarkable specific capacity of ~360 mAh/g with over 100% capacity retention after 500 cycles. This exceptional performance is attributed to a fascinating mechanism change from intercalation to surface pseudocapacitance, triggered by amorphization during cycling. Notably, Li4Ti5O12 does not exhibit any such mechanism change, regardless of the battery cycling conditions.

Driven by the ever-increasing demand and usage of lithium-ion batteries, researchers are continuously striving to advance their performance. While all major components play a crucial role, the anode material's properties are paramount in determining the overall electrochemical performance of a battery cell. In this regard, $Li_4Ti_5O_{12}$ has been favored over graphite due to its minimal volumetric changes. However, it suffers from significant drawbacks such as degassing, low electrical conductivity, and limited specific capacity. This study proposes $TiNbO_4$ as a promising candidate to address these challenges. Operating between a 0-3V potential window, $TiNbO_4$ exhibits a remarkable specific capacity of ~360 mAh/g with over 100% capacity retention after 500 cycles. This exceptional performance is attributed to a fascinating mechanism change from intercalation to surface pseudocapacitance, triggered by amorphization during cycling. Notably, $Li_4Ti_5O_{12}$ does not exhibit any such mechanism change, regardless of the battery cycling conditions.

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Poster Presentation : **ELEC.P-414**

Electrochemistry

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Impact of Lithium Salts on the Electrochemical Performance of Ni-rich Layered Single Crystals

ByungChan Kang, Jin Ho Bang[1,*]

Department of Applied Chemistry, Hanyang University, Korea

[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*

In this study, we investigated the influence of lithium salts on the molten salt synthesis of Ni-rich layered single crystals. Employing Li_2CO_3, Li_2SO_4, and $LiNO_3$, we synthesized crystalline particles ranging from 1 to 2 μm, showcasing impressive control over their size and morphology. Notably, SC-Li_2SO_4 emerged as a champion, exhibiting remarkably reduced grain strain, as revealed by Williamson-Hall plot analysis. This minimized strain proved to crucial, translating into superior material stability. SC-Li_2SO_4 demonstrated exceptional longevity, retaining a remarkable 85% capacity after 100 cycles at 1.0 C, eclipsing its Li_2CO_3 and $LiNO_3$ counterparts (71.2% and 72.9%, respectively). This comparative exploration illuminates the pivotal role lithium salts play in dictating the synthesis and stability of these materials, paving the way for future advancements in this field.

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Poster Presentation : **ELEC.P-415**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Tracking the electrochemical activity of Au@Ag nanoparticles for the nitrite oxidation reaction via single-entity electrochemistry

Gowrisankar Aruchamy, Byung-Kwon Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Nitrite ions (NO2^-) are considered to be an imperative intermediate in biological system and it is widely used as a preservative in water and food industry. However, the excessive liberation of NO2^- ions could cause to the human health and bionetwork. Therefore, sensitive detection of NO2^- ions is still necessary to protect environment. In this work, we describe a novel method for detecting the NO2^- ions via single-entity electrochemistry (SEE) approach using carbon ultramicroelectrode (C-UME). Accordingly, the electrochemical oxidation of NO2^- ions have been achieved by observing the collision of a single Au@Ag core-shell nanoparticle on C-UME with the aid of chronoamperometric method, as depicted in scheme. The variation of transient current signals for Au@Ag core-shell nanoparticles under different potentials, concentrations and volume of analyte was further investigated.

Poster Presentation : **ELEC.P-416**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Investigating Deterioration and Restoration Processes in Anion Exchange Membrane Water Electrolysis Powered by Fluctuating Renewable Energy

Anastasiia Voronova, Sol Kim[1], Bora Seo[2,*]

Hydrogen and Fuel Cell Research Center , Korea Institute of Science and Technology, Ukraine
[1]*Hydrogen and Fuel Cell Research Center , Korea Institute of Science and Technology, Korea*
[2]*Hydrogen and Fuel Cell Research Center , Korea Institute of Science and Technology (KIST), Korea*

Despite significant advancements in low-emission hydrogen production, obstacles related to cost and implementation hinder the widespread deployment of green hydrogen, slowing progress towards achieving a net-zero emissions scenario. Anion exchange membrane water electrolysis (AEMWE) stands out as a promising solution due to its ability to operate flexibly at relatively high loads, allowing for effective integration with renewable energy power. In addition, the availability of cost-effective catalytic materials can significantly reduce the overall system cost. Among economically feasible catalysts for oxygen evolution reaction (OER), NiFe-based materials take the place of one of the most active. Regarding the activity origin, recent studies have highlighted that NiFe-(oxy)hydroxides formed in situ on non-oxide surfaces are effective in enhancing catalyst activity. In this presentation, NiFe-based phosphide was synthesized as OER “pre-catalyst”, followed by the in situ formation of NiFe-(oxy)hydroxide on its surface. The performance of the obtained NiFe-based phosphide/(oxy)hydroxide was evaluated under various loads, including current holding, current cycling, and simulated solar-powered operation. To discern the deterioration and restoration processes, alterations in activation, Ohmic, and mass transport overpotentials, along with the changes in faradaic efficiency and electrochemical surface area were monitored during the operational period. Results indicate that simulated solar operation triggered restoration in all types of overpotentials during zero-load periods, attributed most likely to the dynamically stable dissolution-redeposition process. On the contrary, the performance was not restored

under constant and cycling current operation with short step duration. These findings underscore the importance of zero-load periods in night time for solar-driven operation to facilitate cell performance restoration, resulting in degradation slopes varying between 0.08 and 0.14 mVh^{-1} depending on weather conditions. These insights provide valuable implications for optimizing the AEMWE operating condition under fluctuating renewable energy power.

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Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Unveiling mercury's Electrochemical behavior through Single Entity Electrochemistry

<u>Ganesh Abinaya</u>, Byung-Kwon Kim*

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Mercury is identified as one of the top ten hazardous chemicals by the World Health Organization, raising significant public health concerns. Chronic exposure to such chemicals poses considerable risks to various physiological systems, including the nervous, digestive, and immune systems. Given the ubiquitous presence of mercury in the environment and its potential health impacts on humans, there is a pressing need to monitor its levels within the body. Single Entity Electrochemistry (SEE) emerges as a valuable analytical technique capable of detecting individual particles. SEE demonstrates versatility in analyzing a wide array of substances, ranging from hard particles such as nanomaterials, inorganic and organic composites, and conducting polymers, to soft particles like biological compounds and emulsions. To exemplify, the detection of mercury utilizing Ultramicroelectrode (UME) through electrolysis collision has been successfully conducted, underscoring the efficacy of such electrochemical methods in environmental monitoring and risk assessment.

Poster Presentation : **ELEC.P-418**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Molecular weight determination of Aromatic polymer; Introducing a Novel Approach

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Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Polyether sulfone (PES) is a prominent aromatic polymer renowned for its superior chemical resistance, mechanical robustness, and thermal stability, rendering it indispensable across diverse sectors including aerospace, electronics, and healthcare. Understanding the molecular weight distribution of PES is paramount for tailoring its properties to specific applications. In this study, we present a novel analytical approach leveraging Ultra Microelectrode (UME) technology coupled with cyclic voltammetry (CV) for rapid and efficient determination of PES molecular weight by using Tetracyanoquinodimethane (TCNQ). Our investigation demonstrates a discernible correlation between the molecular weight of PES and the observed steady-state current in cyclic voltammograms. Specifically, higher molecular weight PES samples exhibit a gradual increase in steady-state current because of the π-π stacking of the polymer and redox plays a crucial role in this, providing a direct indicator of molecular weight. Additionally, we establish a relationship between the concentration of polymer end groups and the oxidation current of the redox system, further elucidating the mechanism underlying the observed electrochemical behavior. Compared to conventional methods such as Gel Permeation Chromatography (GPC), Light Scattering, and Nuclear Magnetic Resonance (NMR), our profound electrochemical approach offers distinct advantages in terms of simplicity, reduced time consumption, and ease of use. By circumventing the complexities and resource-intensive nature of traditional techniques, our method presents a promising avenue for expediting the molecular weight determination of PES, thus facilitating the optimization of its properties for various industrial applications

Poster Presentation : **ELEC.P-419**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Improving anion exchange membrane water electrolysis performance using β-NiOOH-encapsulated Ni nanoplates

Mrinal kanti Kabiraz, Sang-Il Choi[1,*]

Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, Korea

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

Hydrogen is considered an alternative energy source capable of replacing fossil fuels and reducing carbon emissions. Anion exchange membrane water electrolyzers (AEMWEs) have demonstrated potential for cost-effective and efficient water electrolysis to generate high-quality hydrogen. However, to improve AEMWE performance, a stable and active nanocatalyst is required for the oxygen evolution reaction (OER) at the anode, a crucial step in electrolysis. Nickel oxyhydroxides (β-NiOOH) grown on the Ni{111} surface have shown favorable activity and stability for OER under alkaline conditions. To further enhance OER stability, we developed Fe-doped nickel nanoplates coated with β-NiOOH (FeNi$\perp\beta$-OOH NPs). These nanoparticles exhibited exceptional OER stability, maintaining a constant current density of 10 mA cm^{-2} for a record-breaking 120 days. AEMWEs fabricated with FeNi$\perp\beta$-OOH NPs/C using the catalyst-coated substrate method achieved a current density of 1000 mA cm^{-2} at 1.81 V, with an energy efficiency of 76.0%. This significant achievement not only demonstrates the potential of FeNi$\perp\beta$-OOH NPs in AEMWEs but also presents new opportunities for cost-effective and high-performance water electrolysis and hydrogen production.

Poster Presentation : **ELEC.P-420**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Improving stability in anion exchange membrane electrolysis using NiFe nanoparticles deposited hydrophilic TiO_2 electrode

Shajahan Shaik, Mrinal Kanti Kabiraz, Sang-Il Choi[1,*]

Department of Chemisty, Kyungpook National University, Korea

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

In this study, the electrochemical deposition synthesis method was used to prepare the NiFe nanoparticles on the TiO_2 nanotubes (NiFe/ATNT) as an efficient oxygen evolution reaction electrode. The NiFe/ATNT electrode exhibited a low overpotential of 235 mV in a half-cell test in 1.0 M KOH solution to reach a current density of 10 mA cm^{-2}. Employing NiFe/ATNT as the anode and commercial Pt/C/ATNT as the cathode, the anion exchange membrane water electrolyzer (AEMWE) achieves a current density of 1670 mA cm^{-2} at 1.80 V, surpassing AEMWE electrolyzer using commercial catalysts (Pt/C/CP ‖ IrO_2/TF). Additionally, it demonstrates remarkable stability for 1500 h at 80 ± 3 °C and 500 mA cm^{-2}, marking the longest observed duration under these conditions in recent studies. The NiFe/ATNT anode, featuring strong metal support interaction and a hydrophilic surface, facilitates fast bubble release, thereby enhancing both performance and long-term stability in AEMWE.

Poster Presentation : **ELEC.P-421**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

New, solid phase ECL coreactant providing high reliability and efficiency in electrochemiluminescence signal

Beom-Jun Shim, **Ik-Soo Shin***

Department of Chemistry, Soongsil University, Korea

Electrochemiluminescence (ECL) is a detection technique that does not require an external light source and offers a higher signal-to-noise ratio and signal sensitivity compared to other spectroscopic analytical techniques such as fluorescence or absorption. In general, ECL generates light through secondary chemical reactions between reaction intermediates resulting from the simultaneous oxidation/reduction of a luminophore by electrical energy. Alternatively, ECL signals can also be generated by using coreactant that boosts excited states of the luminophore through sacrificial chemical reactions. In particular, tri-n-propylamine (TPrA) has been widely used as the coreactant in chemical analysis and biosensing. It facilitates a strong ECL signal of the luminophore even under a mild oxidation potential. However, TPrA's toxicity, hydrophobicity, and chemical instability are constraints to wider applications of ECL, and new coreactants are being actively researched to replace it. We have discovered a new coreactant compound that outperforms the traditional TPrA, which we want to present here. Unlike TPrA, the new coreactant we discovered are water-soluble, solid compounds, stable in air, and provide stronger ECL signaling than TPrA.

Poster Presentation : **ELEC.P-422**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Harnessing the Power of Noble Single Metal Atoms on Carbon Electrodes: A Boosting Charging/Discharging Kinetics in Lithium-Ion Batteries

Jinha Shim, **Jin Ho Bang**[1,*]

Department of Applied Chemistry, Center for Bionano Intelligence Education and Research, Korea

[1]*Department of Chemical & Molecular Engineering, Hanyang University, Korea*

Despite the popularity of single metal atoms (SMAs) in many applications, their utilization in lithium-ion batteries (LIBs) has seldom been explored to date. To examine the potential benefits of SMAs in LIBs, we prepared porous carbons where one of three different noble metals (Au, Ag, and Pt) was embedded in the form of SMAs via a simple galvanic replacement reaction. When exploited as an anode material for LIBs, these SMA-incorporated carbons showed an enhanced capacity compared to control samples that had no SMAs in the carbon network. Our investigation also revealed that the effect of SMAs on the LIB performance depends on the types of metal incorporated, among which Ag SMAs stand out in terms of rate capability and long-term stability. In particular, the Ag SMA-embedded carbon exhibited superior performance even at ultrafast charging/discharging rates, highlighting the unprecedented effects of SMAs as capacity boosters. The reasons for this newly found SMA effect are attributed to the lower interfacial resistances that are induced by delicate modulation of the electronic structure of carbon in the presence of Ag SMAs. This is the first report to harness SMAs for LIBs, which we speculate will open a new frontier in the applications of SMAs.

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Poster Presentation : **ELEC.P-423**
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Improving biodegradable polymer for Melt electrospinning : enhancing conductivity and viscosity with additives

Yun Hyeong Lee, Byung-Kwon Kim[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Biodegradable polymer (BP), produced from renewable resources, find applications in various fields such as biomedical, packaging, textile fibers, and technical items. Despite their remarkable qualities, the high viscosity and low electrical conductivity of BP pose challenges, particularly in the context of Melt electrospinning (MES). Therefore, this research aims to enhance the electrical conductivity and viscosity of melted biodegradable polymers for the melt electrospinning of nanofibers by utilizing various additives. These additives were selected from candidate compounds identified in previous studies. Consequently, this study compares the enhancement in conductivity and viscosity achieved with different additives, with the goal of improving the properties of polymer solutions for efficient nanofiber fabrication. The findings of this research are expected to contribute to the advancement of biodegradable polymer-based nanofiber fabrication techniques and the development of high-performance, sustainable materials applicable across various industries.

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Poster Presentation : **ELEC.P-424**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

NaCl Template-Induced Low-Content Ir Catalyst for Enhancing Cost-Efficiency of Proton Exchange Membrane Water Electrolysis

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Proton exchange membrane water electrolysis (PEMWE) has garnered attention for its high performance, compact design, and fast response to load fluctuations. Developing efficient catalysts for the oxygen evolution reaction (OER) is crucial for advancing the practical application of the PEMWE. However, the necessity of using precious metal-based catalysts such as iridium (Ir) and ruthenium (Ru) in acidic media increases the overall cost of PEMWE stack. To address this issue, various strategies have been explored to produce low-content Ir catalysts, including structural modifications to increase surface area or utilizing low-cost, electrochemically stable metal oxide supports, yet their performance remains unsatisfactory. In this presentation, we present a synthesis strategy for tin oxide-supported iridium oxide (IrO_x/SnO_y_NaCl) catalyst, prepared using NaCl as a structure control template to reduce IrO_x particle size and tune its electronic structure. The IrO_x/SnO_y_NaCl catalyst exhibited a high OER activity, comparable to that of state-of-the-art Ir-based OER catalysts. Electrochemical and X-ray spectroscopic characterization confirmed that the IrO_x/SnO_y_NaCl catalyst has a large surface area and a mixed valence state of Ir^{3+} and Ir^{4+}, known to be favorable for OER. It indicates that the use of NaCl template increases the catalytic activity by enhancing the dispersion of IrO_x nanoparticles and tuning the electronic structure. Furthermore, in situ spectroscopic characterization validated that the use of NaCl and SnO_2 support promotes the oxidation state transition of Ir species in the catalyst, thereby enhancing OER activity. Notably, the IrO_x/SnO_y_NaCl catalyst showed a high single-cell performance for PEMWE, achieving 2.6 times higher mass activity than that of commercial IrO_2 catalyst. These results highlight the potential of the proposed catalyst synthesis strategy to significantly enhance the cost-efficiency of PEMWE system.

Poster Presentation : **ELEC.P-425**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Unveiling the Critical Role of Crystallinity in Photogenerated Hole Tranfer Behavior of TiO_2

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Titanium dioxide (TiO_2) is one of the excellent semiconductor materials for photoelectrodes due to its high light conversion efficiency and remarkable chemical stability. However, its photoelectrochemical (PEC) performance is heavily influenced by subtle changes in surface properties, which vary depending on its crystallinity. This study explores the PEC behavior of photoelectrodes made of both single- and polycrystalline TiO_2 in the presence of acetoamido-2,2,6,6-tetramethylpiperidine-1-oxyl free radical (ACT) as a mediator in acetonitrile. Photoelectrochemical impedance spectroscopy provides deeper insights into the charge transfer and recombination kinetics under the influence of surface defects. The results reveal unprecedented PEC behavior in polycrystalline TiO_2, suggesting an anomalous hole transfer mechanism driven by surface trap states facilitated by the ACT mediator. The study further proposes the intriguing potential of charged acetonitrile as a hole scavenger, supported by analyses using scanning electron microscopy, energy dispersive X-ray spectroscopy, and Raman spectroscopy.

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Poster Presentation : **ELEC.P-426**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Active phase formation in lithium cobalt oxide via potential-driven reconstruction for improved oxygen evolution reaction

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Dynamic self-reconstruction of electrocatalysts occurs heterogeneously in terms of depth and spatial distribution. It results in non-uniformity of phase distribution, which is crucial for designing highly efficient electrocatalysts. Here, we investigate the phase evolution of $LiCoO_2$ (LCO) based on the control of the potential window for the oxygen evolution reaction (OER) through multi-scale analysis. We demonstrate that LCO delithiation can be initiated near the OER potential of 1.8 V_{RHE} with further propagating from the surface to the core particles with cycling. Our Raman line scans and phase maps reveal that β-CoOOH formation is induced through delithiation at OER potential. Furthermore, β-CoOOH species having depths of hundreds of nanometers exhibit enhanced OER activity. Our results establish that a simple cycling potential window-controlled strategy is an effective approach for creating highly active OER catalysts, and based on these findings, we can provide in-depth insights into the self-reconstruction process.

Poster Presentation : **ELEC.P-427**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Flow Synthesis of Ketones from Benzylic Methylenes via Electrooxidative C-H Activation

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Benzylic ketones generated through the oxidation of benzyl C-H bonds have received significant attention as building blocks for pharmaceutical synthesis across various fields. Among various methods, electrochemical synthesis methods have been widely used for the advantage of being able to react in an environmentally friendly manner using electrical energy without oxidants and reductants. However, conventional batch system has the disadvantage of long reaction times and peroxidation, so various research on electrochemical synthesis through a continuous flow system has been reported. Therefore, we proceeded with the direct oxidation of the C–H bond of benzyl methylene via continuous flow electrochemical synthesis. Continuous flow electrochemical reactions, which possess a higher surface area-to-volume ratio than traditional batch reactions, can reduce peroxidation and enhance reaction efficiency with lower currents and shorter reaction times. With this electrochemical continuous flow synthesis, satisfactory yields of benzylic ketones could be obtained under milder conditions, more effectively, and in a shorter time.

Poster Presentation : **ELEC.P-428**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Sustainable eco-friendly NaCl salt powder-assisted method to synthesize SiO_x/C as anode materials originated from rice husk for lithium-ion batteries

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Silicon oxide (SiO_x) anode with higher specific capacity than conventional graphite and better capacity retention than pure Si attracted significant attention from both academia and industry. However, synthesizing nanostructured SiO_x typically requires toxic precursors and complicated procedures. Herein, a green and facile synthesis for the preparation of rice husk-derived SiO_x/C composite was introduced based on the salt-assisted method. During synthesis, the NaCl salt not only served as a physicochemical activation agent but also facilitated catalytic graphitization and amorphous silica formation. The SiO_x/C anodes exhibited a high initial charge/discharge capacity of 422.05/915.93 mAh g^{-1} at 0.05 A g^{-1} current density and stable cycling performance over 500 cycles. In addition, the SiO_x/C composite produced by the sub-micron NaCl crystal powder-assisted method delivered better rate capability and facile kinetics than the SiO_2/C composite which was prepared without salt.

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Poster Presentation : **ELEC.P-429**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Comparison of the mediator's electrochemical characteristic with different carbon chain length

Jihyuk Kim, Hyug-Han Kim[1,*]

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In the electrochemical seonsor field, we studied about differences in the carbon chain length of the mediator which transfers electrons from glucose to the electrodes by glucose dehydrogenase(GDH). The hydrophobic Poly(4-vinylpyridine) (PVP), which has a molecular weight 160,000, were quaternized with Bromoacetic acid and 10-Bromodecanoic acid to synthesize a hydrophilic polymer. And then, an Osmium complex having an amine group as a ligand was combined this polymer by EDC and NHS, and used it as a new mediator of the electrode. The structure of synthesized polymer was examined by FT-IR, 1H-NMR, and its electrocheimal charteristic was examined by cyclic voltammetry(CV) and Zeta potential. Lastly, the electrochemical difference according to the length of the carbon chain was confirmed by comparing the quantitative reaction of each mediator by glucose concentration through CV. The results showed that the mediator of long carbon chain polymer has a better electrochemical performance than short one.

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Poster Presentation : **ELEC.P-430**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Development of a new electron mediator applicable to enzymatic biofuel cell

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In this study, we aim to develop a new electron mediator applicable to enzymatic biofuel cells using enzymes. Using osmium, a Group 8 metal element, as a central element, 4,4'-Bis(N,N-dimethylamino)-2,2'-bipyridine(DMAB) as a ligand, a new electron mediator was developed by synthesizing a 4 coordination organometallic complex. In addition, for stability and water solubility on the enzymatic biofuel cell electrode, a five-coordinate complex was formed using polyvinyl imidazole (PVI) To check the oxidation catalyst current of the developed electron mediator, FAD-GDH enzyme and glucose were mixed and a test was performed for each glucose concentration through cyclic voltametry. Through this, it was confirmed that the newly developed electron mediator of the organometallic complex can be applied to an enzymatic biofuel cell.

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Poster Presentation : **ELEC.P-431**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Effect of Capping Agent for Pt/Cs on Stability of Electrochemical Toluene Hydrogenation

Jueon Park, Ara Jo[*]

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Liquid Organic Hydrogen Carriers (LOHC) are reusable materials for storing and transporting hydrogen, enabling its utilization without carbon dioxide emissions. In this study, toluene was electrochemically hydrogenated to methylcyclohexane using various Pt/Cs as catalysts. While commercial Pt/C (cPt/C) catalysts are well known for their effectiveness in aqueous applications such as water electrolysis and oxygen reduction reactions, finding alternatives with improved activity and durability remains challenging. We observed a significant decrease in durability when the cPt/C was employed in a non-aqueous system. To investigate this, our group focused on the surface properties of the catalysts and synthesized Pt/C catalysts with and without citrate ions, because the presence of surfactants was identified as the primary difference between commercial Pt/Cs and in-house Pt/Cs. Interestingly, the synthesized catalyst without citrate showed better stability than other catalysts that contain the capping agent in non-aqueous media but exhibited a less stable performance for oxygen reduction reaction in aqueous media. TEM analysis revealed a correlation between catalytic activity and Pt nanoparticle aggregation during the hydrogenation. By comparing the properties of Pt/Cs with various functional groups, this work proposes a new guideline for the development of electrochemical catalysts for non-aqueous systems.

Poster Presentation : **ELEC.P-432**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Electrochemical Measurements of the Surface Area for Platinum Electrodes

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As researches in the field of energy and environment expand with the advancements in nanotechnology, the importance of electrochemical characterization of materials is increasing. Generally, the electrochemical properties are normalized with the surface area of the electrodes to assess the intrinsic performance of the electrode materials. This normalization has been achieved using electrochemical surface area (ECSA) and geometric surface area (GSA), and among them, the ECSA reflects the roughness and porosity of the electrode surface. Therefore, the estimation of the ECSA value of the electrode is crucial to interpret the innate characteristics of materials. The ECSA was routinely assessed based on electrochemical phenomena such as hydrogen adsorption/desorption, metal underpotential deposition (UPD), and double-layer capacitance, each resulting in different chemical reactions due to variation in the materials forming a monolayer on the electrode surface. In this study, we examined the ECSA values of a platinum disk electrode (Pt) and Pt deposited-glassy carbon electrode (Pt/GC) using the aforementioned methods. Our works provided an overview of the theoretical merits and limitations of each measurement technique and emphasized the importance of understanding potential experimental shortcomings in the electrochemical experiments to enhance the reliability of ECSA estimation.

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Poster Presentation : **ELEC.P-433**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Electrochemical Hydrogenation of Toluene using Various Metal/C Catalysts

Sunhyung Han, Ara Jo[*]

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The hydrogenation of Liquid Organic Hydrogen Carriers (LOHC) serves as a promising method for mitigating the concern regarding high flammability and gaseous nature of hydrogen during storage and transportation. Electrochemical hydrogenation enables the formation of organic molecules containing sufficient hydrogen at room temperature and ambient pressure. However, research on catalysts for LOHC hydrogenation, excluding noble metal-based catalysts has not been actively studied. In this work, we synthesized various catalysts not only single metals such as Ru, Pd, Ir, and Pt, but also Ru-based alloys doped onto a carbon black. Electrochemical hydrogenation experiments were conducted using toluene as a LOHC. The stability of the catalysts was assessed by electrochemical measurement while the Faradaic efficiency (FE) of the conversion from toluene to methylcyclohexane was determined via gas chromatography analysis. As a result, our findings reveal that catalysts comprising alloys of Pd and Fe, in conjunction with Ru demonstrated improved FE and reduced overpotential, respectively. This work suggests the potential of the alloy catalysts in achieving high efficiency for toluene hydrogenation applications.

Poster Presentation : **ELEC.P-434**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Concentration Effect of Redox Molecules on Electrochemical Reaction in Nanoporous Electrodes

Hyun Ju Yang, Junhee Yu, Hyo Chan Lee, Je Hyun Bae*

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

Nanoporous electrodes have been extensively utilized in the fields of energy conversion, sensors, and catalysts owing to their high surface-to-volume ratio. The effect of the nanoporous structure rather than the increase in the surface area has attracted significant attention in both fundamental studies and enhanced applications ofnanoporous electrodes. The unique phenomenon exhibited by the nanoporous structure, which is not seen in flat electrodes, is called nanoconfinement effect. In this study, we explore the effect of concentration of the reactant species on the nanoconfinement effect at the nanoporous electrode. The effect appears differently depending on the degree of adsorption and charge of the redox molecules. These findings may provide an insight into electrochemical analysis and electrocatalysis based on nanoporous structures.

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Poster Presentation : **ELEC.P-435**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Effect of Electric Double Layer Overlapping on Electrochemical Reactions at Nanoporous Electrodes

Hyo Chan Lee, Hyun Ju Yang, Junhee Yu, Je Hyun Bae[*]

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

In this study, we investigate how electrochemical reactions can be influenced by overlapping electric double layers (EDLs) in nanoporous electrodes. When a potential is applied to an electrode immersed in an electrolyte solution, ions with charges opposite to that of the electrode accumulate around it, forming an EDLs. Unlike flat electrodes, when the pore size is comparable to the thickness of the EDLs, the EDLs overlap in the nanoporous electrode so that electrochemically effective surface area is not the same as that of the real electrode surface. While previous research has primarily focused on the charging behavior of ions in nanoporous electrodes, the impact of EDLs overlapping on Faraday reactions has received less attention. Through chronoamperometry and voltammetry experiments, we demonstrate that electrolyte concentration, measurement time, and overpotential are key factors influencing electrochemical reactions due to EDLs overlapping. These findings shed light on the potential applications of nanoporous electrodes in catalysis and sensor technology

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Poster Presentation : **ELEC.P-436**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Operando Li Imaging: Elucidating lithium transport associated with internal strain-stress in individual NMC particles affected by interface conditions in polymer electrolyte

Junho Bae, Jongwoo Lim*

Division of Chemistry, Seoul National University, Korea

Solid electrolytes in all-solid-state batteries (ASSBs) have attracted attention due to their high energy density. However, their interface stability remains a challenge compared to liquid electrolytes, with a significant gap in understanding the differences in lithium transport behavior under these distinct interfacial environments. Conventional analyses have struggled to isolate mechanisms due to the ensemble effect in the composite electrode, lacking studies on the real-time measurement of individual single particles. This research introduces a novel platform based on X-ray microscopy to analyze lithium-ion transport in single NMC particles, comparing those coated with LiNbO3 against uncoated counterparts. The study reveals that particles with enhanced interface stability through coating exhibit uniform lithium diffusion behavior akin to that in liquid electrolytes, unaffected by electrolyte side reactions. In contrast, particles with poor interface stability showed gradual surface deterioration, further affecting lithium-ion diffusion adjacent to the degraded area. The degradation previously attributed only to surface deterioration and mechanical damage is also significantly affected by internal stress-strain induced by side reactions, leading to reduced capacity. These findings underscore the critical importance of interface stability in ASSBs, suggesting avenues for further research and development in this field.

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Poster Presentation : **ELEC.P-437**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Bioelectrocatalytic nitrous oxide reduction to ammonia

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Nitrous oxide is a substance with a greenhouse effect approximately 300times greater than that of CO_2. It is primarily generated during the incineration of sludge, a collection of pollutants treated in sewage treatment plants. The atmospheric concentration of nitrous oxide reached 333ppb in 2020 and is increasing by approximately 1ppb annually.Therefore, it is crucial to capture and treat N_2O in sewage treatment plants. However, the complex and costly property of the treatment process necessitates exploring alternative methods, such as utilizing nitrous oxide reductase(nosZ) through bioelectrocatalysis, for a simpler and more cost-effective conversion to harmless N_2.Also, another enzyme, nitrogenase catalyzes the synthesis of value-added compounds NH_3 by utilizing N_2. Nitrogenase utilizes reducing agent and biological energy (ATP) to convert N_2 into NH_3. However, bioelectrocatalysis can replace the reducing agent with the electrode, enabling sustainable ammonia production.Combine these two processes; N_2O to N_2 by nitrous oxide reductase and N_2 to NH_3 by nitrogenase. Using the enzyme cascade system concept ultimately allows for the conversion of nitrous oxide into the ammonia. Hydrogen(H_2) is a key element in future energy projects. However, gaseous hydrogen, due to its combustible and explosive nature, presents difficulties in storage and transportation. Therefore, NH_3, which can be compressed in liquid form, is a much more stable material, so it is suitable for hydrogen storage and transportation. Consequently, we will utilize bioelectrocatalysis to convert the atmospheric pollutant nitrous oxide into ammonia through an enzyme cascade.

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Poster Presentation : **ELEC.P-438**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Mediated Enzymatic Bioelectrocatalysis for highly efficient NADH regeneration and bioinspired redox flow battery

Jeon Yerin, Hyenseong Ju[1], Geum Nahui[2], Yoo Seok Lee[2,*]

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Nicotinamide adenine dinucleotide (NAD^+) and the reduced form of it (NADH) are cofactors that act as electron acceptors and donors that facilitate energy and materials conversion under mild conditions. They are also utilized as substrates in about 80% of oxidoreductases. In particular, NAD^+, an electron donor, should be regenerated so that enzymes can continue to convert energy and materials during metabolic reactions. We constructed an efficient bioelectrocatalytic NAD^+ regeneration system by using neutral red(NR), a small and diffusible redox active molecule, as a mediator to transfer electrons between the redox center of the enzyme catalyst and the electrode. NR acts as an electron acceptor for NADH with a similar redox potential, minimizing thermodynamic and kinetic energy losses in the electron transfer process. In this study, to achieve more efficient NAD^+ regeneration, diaphorase, one of the NADH dehydrogenases, was insulatingly immobilized on carbon cloth, a high areal density electrode, for mediated electron transfer(MET). The use of mediators results in higher current density than other methods because they interact with all the enzymes immobilized on the electrode. All immobilized diaphorases react with the substrate in the electrolyte to catalyze the electron transfer from NADH to NR, and the reduced NR mediates the NADH-derived electrons to the electrode through direct interaction with the electrode and is finally oxidized. These MET-based NAD^+ regeneration system binds to various enzymes that reduce NAD^+ to NADH, thus completing the pathway of energy and material transfer. Our regeneration system can be used as a method for regenerating redox couples such as NAD^+/NADH to provide redox power in enzyme-enabled Bio-inspired Redox Flow batteries.

Poster Presentation : **ELEC.P-439**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Stable and high-sensitivity enzymatic biosensor capable of phenol measurement based on nanostructured bioelectrodes using block copolymer lithography

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[1]*Department of Chemical Engineering & Biotechnology, Tech University of Korea, Korea*

Soil and water pollution are serious due to artificial chemicals such as pesticides, pharmaceuticals, and dyes. In particular, phenolic compounds are industrial wastes that are highly carcinogenic and toxic and pose a significant risk to human health when exposed. Therefore, developing a tool capable of monitoring phenol analysis, an environmental pollutant, is crucial to ensure sensitivity and reliability. Enzyme-based biosensors offer ease of use for phenol concentration monitoring, detecting the target analyte sensitively through specific reactions. Moreover, efficient analysis of phenol concentration is achievable by manufacturing enzyme-based biosensors utilizing the high electrical conductivity and catalytic efficiency of gold (Au) particles. A crucial aspect affecting the performance of enzyme-based biosensors is ensuring that the enzyme does not aggregate on the electrode and remains stably fixed. In this study, to enhance adhesion between Au and the electrode, block copolymer lithography is employed to pattern the electrode, followed by coating with Au particles. Increasing the electrode's surface area using Au particles prevents enzyme aggregation and promotes stable enzyme fixation, thereby maintaining enzyme stability. Furthermore, the large surface area of the electrode is vital as it enhances electron generation during the enzyme's target reaction, thereby increasing electron transfer efficiency. Lacase, an enzyme that oxidizes phenolic hydrocarbons, can be fixed by crosslinking with glutaraldehyde. By proposing nano- and micro-structured electrodes and utilizing electrode modification with Au particles for stable enzyme fixation, high-efficiency phenolic measurement biosensors can be manufactured.

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Poster Presentation : **ELEC.P-440**
Electrochemistry
Exhibition Hall 2 FRI 11:00~13:00

Development of stretchable electrode based on metal nano fibers with improved elasticity through wrinkle structure

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Recently, there has been a rapid surge in the development of stretchable devices. Stretchable electrodes, which play a crucial role in enabling the functionality of these devices, are being explored using various materials such as carbon nanotubes, graphene, and metal nanomaterials. While carbon nanomaterials like carbon nanotubes and graphene exhibit excellent conductivity, their production processes are complex, and structural deformation can lead to increased resistance and costs. Additionally, thin metal films are prone to cracking and experience mechanical strength deterioration with repeated use. Although metal nanowires show promise, they face challenges such as contact resistance and unstable junctions between wires. The introduction of stretchable sensors utilizing metal nanofibers fabricated through electrospinning presents a promising solution. Metal nanofibers fabricated via electrospinning are relatively easy to fabricate and offer excellent electrical conductivity due to their high aspect ratio. However, their mechanical strength is weak due to poor adhesion to the substrate. To address these limitations, a method has been developed to anchor conductive nanofibers into bilayer polymer wrinkles. This approach aims to enhance the mechanical strength of stretchable electrodes by strengthening the adhesion between conductive nanofibers and the substrate. With these advancements, stretchable electrodes demonstrate excellent electrical properties along with high mechanical strength. This innovation opens up potential applications in various fields, including wearable devices, medical monitoring systems, and human-machine interfaces.

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Poster Presentation : **ELEC.P-441**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Direct/Mediated electron transfer based bioelectrocatalytic NADH regeneration for enzymatic biofuel cell

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NADH is a coenzyme found in living cells and transports electrons from one reaction to another, playing an important role in cell metabolism by promoting numerous biochemical processes. NADH is oxidized to NAD+ during these reactions, and NAD+ must be regenerated to maintain the supply of NADH in order for cell metabolism to continue efficiently. Types of enzymes are classified into metal catalysts and non-metal electrocatalysts depending on cofactors. However, it requires expensive costs to use metal redox materials and cannot be regenerated. Therefore, bioelectrical catalysts, which are biological catalysts, are used as an alternative to metal electrocatalysts to catalyze the electrochemical reaction on the surface of conductive electrodes. In this study, a small and diffuse redox active molecule, Neutral Red, was used as a mediator to move electrons between the center of enzyme redox and the electrode, and in order to increase the current density of an enzyme-based bioelectrocatalyst system, diaphorase, an enzyme having redox enzyme activity, and Carbon cloth, an electrode with a high surface area, were used to create a mediated electron transfer-based bioelectrode. The high surface area bioelectrode improves the current density in a small geometric area, resulting in the miniaturization of bioelectrical catalyst platforms such as biosensors and biofuel cells. In this study, NADH regeneration is explained using the mediator electron transfer between the electrode and the diphorase, and this conceptual development has the potential as a cost-effective and sustainable energy storage solution that promotes the development of next-generation energy technology.

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Poster Presentation : **ELEC.P-442**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Laser-induced graphene (LIG) based Electrochemical Sensor for the Colorimetric detection of Glucose

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Demand for wearable sensors that can be attached to the human body and are suitable for point-of-care (POC) and real-time analysis has been increasing recently. One of the ways to make this possible is by using flexible electrodes based on laser-induced graphene (LIG), which has the advantage of one-step manufacturing and customization. Also, whereas most electrochemical biosensors require additional display devices to read the electrochemical signals, using the colorimetric method would allow the observation of signals with the naked eye. In this work, we developed a LIG based colorimetric electrochemical sensor, using the bipolar electrode (BPE) configuration. For the electrochromic material we used polyaniline (PANi), which has a wide color range, and to observe the color change clearly we formed indium tin oxides (ITO) particle layers. The other side of the bipolar electrode was modified with catalytic materials such as Prussian blue (PB) and glucose oxidase (GOx) to generate electrochemical signals according to the glucose concentration. As a result, we developed a flexible electrochemical sensor that display color changes depending on the amount of glucose.

Poster Presentation : **ELEC.P-443**

Electrochemistry

Exhibition Hall 2 FRI 11:00~13:00

Highly efficient Enzyme cascade based Bioelectrocatalytic CO_2 conversion and PHB synthesis.

Junsup Shin, Bae Jaesung, Yoo Seok Lee[*]

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The costly nature of reduced nicotinamide adenine dinucleotide (NADH) and its stoichiometric requirement in polyhydroxybutyrate (PHB) synthesis necessitate the efficient regeneration of NAD^+ into NADH. Common NADH regeneration methods rely on enzymatic reactions using NAD-dependent dehydrogenases or employ photochemical/electrochemical techniques. However, these approaches may result in the undesired formation of inactive NAD_2 dimers. To address these challenges, we propose a bioelectrocatalytic approach that integrates enzymatic and electrochemical techniques for effective NADH regeneration. The method utilizes a modified carbon based electrode capable of regenerating NADH and reducing acetoacetyl-CoA. This electrode serves a dual role in NADH regeneration and CO_2 conversion, presenting a sustainable and efficient method for PHB synthesis. The experimental design leverages the synergies of enzymatic and electrochemical processes, offering a promising alternative to conventional NADH regeneration limitations. The electrode's multifunctionality enhances NADH regeneration efficiency, facilitating multiple system runs with an initial NADH dose and aiding in CO_2 conversion.

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Poster Presentation : **EDU.P-414**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Development and pilot application of a non-residential camp-style ‘Planning a science exhibition’ program for elementary science-gifted students

Hunsik Kang

Gifted Education, Seoul National University of Education, Korea

This study developed and piloted a non-residential camp-style field trip program called "Planning science exhibition" for elementary science-gifted students. The program consists of three phases: pre-visit, main-visit, and post-visit, each lasting one day. The pre-visit consists of introducing the task, exploring a science museum exhibits, deciding on a theme for the science exhibition and planning the exhibition, and exploring the science museum in online. During the main-visit, you will visit the science museum and collect the necessary materials. The post-visit consists of finalizing the theme of the science exhibition, creating an exhibit layout and promotional materials for the science exhibition, presenting the planned science exhibition, and sharing perceptions of the program developed in this study. The program was piloted with students at a science-gifted education center in Seoul, and their perceptions of the program were investigated. Many elementary science-gifted students had various positive perceptions of the program in terms of various cognitive and affective aspects, and some students mentioned the limitations of the program.

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Poster Presentation : **EDU.P-415**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Development of Middle School Science Creative Quiz Applying Elements of Gamification

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The purpose of this study is to develop science creativity quizzes that applied gamification elements in order to providing not only a tool to check achievement in science during the self-study semester for first-year middle school students but also a positive direction for improving students' interest and academic abilities in science. In addition, it helps determining their future career paths. Based on the prior study, which is developed the creative quizzes for the first-year high school chemistry unit, the quiz types are classified into five categories such as; (1) a type to find regularity in number/letter arrangement, (2) a type to find regularity in picture arrangement, (3) a type to use of sticks and matchsticks, (4) a type of logical reasoning and language play (letter combination), (5) a type of culprit finding. And total 78 quizzes are developed for the first year of middle school each science unit curriculum, reflected elements for gamification and scientific creativity components defined in previous research. In addition, developed with leveling at least 3 quizzes per subunit in connection with the unit goals and achievement standards. Through the developed creative quizzes, students can improve scientific creativity elements such as unusual thinking, consistency and associational thinking. And in order to improve their interest and concentration in class, the gamification elements mainly used in the quiz operation was compete such as points, levels, and rankings, but challenge, reward, and relationship elements were also used appropriately. Through this study, the quizzers can be developed utilized to fit the content of other units so that the quiz development process is presented. In addition, the developed quizzes can be used in various teaching and learning situations such as science classes, mentoring, educational processing, club activities, schools, and elective situations for first-year middle school students and above. And it can also be used in situations to find not only Improving creativity, causing interests/curiosity but also concentrating.

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Poster Presentation : **EDU.P-416**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Service Learning Experiences of Pre-service Science Teachers at Chosun Space Lab STAR Bridge Center

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The STAR Bridge Center, funded by the Korea Foundation for the Advancement of Science & Creativity, serves as a vital link between cutting-edge advancements in science and technology and education for elementary, middle, and high school students, as well as teachers. The Chosun Space Lab STAR Bridge Center has developed programs for science learning in schools. These programs offered activities tailored to each school level, including space satellite projects and exploration using LEGO coding for elementary school students, video satellites using Raspberry Pi for middle school students, and communication cube satellites using Arduino for high school students. The developed science learning program served as the foundation for in-service teacher training programs and career exploration activities for elementary and secondary school students. Pre-service science teachers participated in the in-service teacher training program as assistants, collaborating with teachers on how to integrate satellite-related experiments and computer software programs into their teaching methods. Additionally, in student career exploration activities, pre-service teachers acted as mentors, guiding elementary and high school students in space technology-related exploration activities and career exploration, drawing from their experiences gained during teacher training. Through the STAR Bridge center programs, pre-service science teachers experienced the latest science and technology, explored ways to apply it in their classrooms, and enhanced their professional skills through mentoring students. STAR Bridge Centers are operated by a team of scientists, teachers, pre-service teachers, and students, providing pre-service teachers with a meaningful and enriching volunteering experience in education.

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Poster Presentation : **EDU.P-417**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

[Withdrawal] The study of Science Communicators' competencies in their curriculums

GeunHyung Lee

Pusan National University, Korea

Poster Presentation : **EDU.P-418**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Comparison of Attitudes Toward Chemistry Between Science Camp Participants and Regular Students

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The purpose of this study is to compare the attitudes toward chemistry between students who participated in a science camp and regular students. For this, 70 students (25 elementary, 18 middle, and 27 high school students) who expressed a willingness to voluntarily participate in a science camp conducted by K University in South Chungcheong Province, and 75 regular students (25 elementary, 20 middle, and 30 high school students) from the same region were examined for their attitudes toward chemistry.The assessment tool used was an adapted questionnaire from previous studies and a 5-point semantic differential scale consisting of 20 pairs of adjectives related to attitudes toward chemistry, with adjusted Likert steps. Students participating in the science camp completed the paper-based survey before joining the camp's programs, while regular students were facilitated to respond to an online survey under teacher guidance. Responses from students who did not answer sincerely were excluded. To analyze the attitudes toward chemistry among all students, a paired sample t-test was performed, and a non-parametric test was used to examine differences by school level. The results are as follows: First, a statistically significant difference in attitudes toward chemistry was observed among all students based on whether they actively participated in science activities. Second, a significant difference in attitudes toward chemistry was noted between active participants in science activities and regular students within the same school levels.

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Poster Presentation : **EDU.P-419**
Chemistry Education
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Deriving a Paradigm Model for Enhancing the Pedagogical Competence of Pre-service Chemistry Teachers Experiencing the Teaching Practicum Semester System

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The purpose of this study is to explore implications for enhancing the teaching professionalism of pre-service chemistry teachers who participated in the Teaching Practicum Semester System pilot application. To achieve this, in-depth interviews were conducted with pre-service chemistry teachers, cooperating teachers from the practicum schools, and curriculum education professors, aiming to derive key elements for enhancing the teaching professionalism of pre-service chemistry teachers in the Teaching Practicum Semester System program. Individual interviews with pre-service science teachers lasted approximately one hour each for two sessions, while joint interviews with cooperating teachers and curriculum education professors involved in the integrated practicum courses were conducted for approximately two hours each for two sessions. In-depth interview questions were structured based on the experiences during the one-month observation period and three-month teaching demonstration period of the first semester of the Teaching Practicum Semester System. Approximately 25 questions were asked, including, 'Why do you think prompting was used most frequently in classroom discourse?' Discussions were held based on the responses to these questions, and follow-up questions were asked as necessary. All in-depth interviews were recorded and transcribed, and data analysis was conducted using grounded theory methods. Through open coding of the data, a total of 80 concepts, 25 sub-categories, and 15 categories were identified. Axis coding was then conducted based on the relationships among the categories identified through open coding. Based on this, a paradigm model was proposed, utilizing causal conditions, contextual conditions,

central phenomena, mediating conditions, action/interaction strategies, and outcomes of the identified categories.

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Poster Presentation : **EDU.P-420**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Analysis of the effectiveness of the chemical virtual laboratory program for high school students in disadvantaged areas

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In this study, online science virtual laboratory contents were developed and applied to high school students indisadvantaged areas. Through this, the purpose is to verify the effectiveness of applying laboratory contents for online science in chemistry classes of high school students. In particular, we tried to verify the effectiveness of the program through changes in students' affective attitudes in the learning process. The program used 'molecular model virtual laboratory' and 'acid and base neutralization proper virtual laboratory' contents developed by the Korea Institute of Science and Technology Information (KISTI). A virtual experiment manual was developed and teacher training was conducted so that field teachers could conduct classes. Participants are high school students in the laboratory class who are applied to the newly developed online science virtual laboratory program. A self-report questionnaire was conducted before and after the application of the program to measure the degree of change in the science positive experience index. The data were analyzed by descriptive statistics and corresponding sample using SPSS 27. As a result of the study, it was found that students who were applied to the online lab program significantly increased their science learning emotions, science-related self-concept, science learning motivation, science career abandonment, and science-related attitudes after the program was applied. Meanwhile, as a result of analyzing the change in the gender positive experience index of science among students in the experimental class who received the program, the pre-post difference for female students was found to be more significant than that for male students. Based on these results, it is expected that the gap in learners' academic background according to regional and school conditions and educational environments can be bridged by developing online science virtual laboratory learning models

and programs. In addition, through the integration with convergence education, implications for diversification of content topics and contents, and edu-tech teaching and learning methods were obtained.

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Poster Presentation : **EDU.P-421**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Developing a TPACK training programme for science teachers and analysing its effects

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The purpose of this study is to develop a training programme to develop TPACK in science teachers and to analyse its effects. To this end, the concepts of TPACK and its components PK, CK, TK, PCK, TPK, and TCK were summarised. Then, the sequence and pathways through which TPACK can be developed were investigated to provide a basis for programme development. In addition, evaluation criteria for TPACK, PK, CK, and TK were extracted to analyse their effects. The developed training programme consisted of five stages of awareness, acceptance, application, exploration, and development, with a pathway that integrates the three domains by developing PK and CK first, followed by TK. In terms of content, PK was taught through responsive teaching, CK was taught through models and model ignorance, and TK was taught through scratch programming. The training programme was delivered in 12 two-week sessions to 18 in-service science teachers enrolled in a graduate school of education. The effects of the programme was measured in each of the five dimensions of TPACK: active/constructive/practical/intentional/collaborative. The average of the total score of each dimension was significantly improved from 5 to 9 points. In addition, the levels for PK, CK, and TK each improved significantly. This study highlights the importance of TPACK developmental training programmes for teachers and provides a systematic approach that can contribute to improving the quality of education for teachers and students. In particular, the study provides criteria for assessing teachers' TPACK, which will provide teachers with the opportunity to diagnose and develop their own professional development, and will be useful to teachers and education professionals through practical guidelines and materials for TPACK development in the classroom.

Poster Presentation : **EDU.P-422**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Exploring Effective Elimination Strategies for "Killer Items" in the Chemistry I of the Korean College Scholastic Ability Test (CSAT)

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The number of students choosing Chemistry I in the CSAT has been steadily decreasing. Among the various factors contributing to this decline, the high difficulty level of the so-called "killer items" is considered a significant obstacle. Fortunately, the Ministry of Education announced the exclusion of killer items from the CSAT in June 2023. This study aims to identify the characteristics of killer items and analyze their impact on test difficulty. By comparing Chemistry I items from the 2022 and 2023 CSATs, as well as the 2024 June and September mock exams and the 2024 CSAT, this research investigates the changes in item difficulty before and after the announcement of killer item exclusion. Based on the findings, this study proposes effective strategies for eliminating killer items from the Chemistry I of the CSAT.

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Poster Presentation : **EDU.P-423**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Changes in the Perception of Artificial Intelligence among Pre-service Chemistry Teachers through an Educational Program Utilizing Generative Artificial Intelligence

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In this study, we sought to identify and analyze how prospective chemistry teachers' perceptions of artificial intelligence change through educational programs utilizing artificial intelligence. To this end, an educational program was implemented to utilize artificial intelligence and design and practice classes using artificial intelligence for 17 prospective chemistry teachers at a teacher's college in North Chungcheong Province. Pre-service chemistry teachers' perception of artificial intelligence was divided into three categories: accessibility of artificial intelligence, possibility of replacing human jobs with artificial intelligence, and creativity of artificial intelligence. This was prepared through pre- and post-survey data and outputs from pre-service science teachers' educational programs. Changes in the perception of chemistry teachers were confirmed. Through this, we hope to derive points to keep in mind when using artificial intelligence in education.

Poster Presentation : **EDU.P-424**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

An Analysis of the Self-Assessments in the Matter Units of Elementary Science Textbooks for 3rd Grade Developed Under the 2015 Revised National Curriculum

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In this study, we analyzed the self-assessments presented in the matter units of elementary science textbooks for 3rd grade developed under the 2015 revised national curriculum. The analytic framework, which consist of positions, targets and contents, response types, assessment standards, references, production of assessment criteria, and feed-backs, was developed based on previous studies. The analyses of the results revealed that there were many self-assessments in the assessment areas of the textbooks, which shows a similar pattern to the traditional result-oriented assessments. Some publishers, however, presented self-assessments in the body texts and the introduction of the units. Targets and contents of self-assessments were mainly knowledge and competence of students, while attitude was relatively less assessed. As for the response types of self-assessments, self-rating was most common. Furthermore the publishers tended to present specific response types. None of the publishers presented assessment standards and references for self-assessments. Feed-backs were only utilized in limited ways by a few publishers. In addition, the production of assessments criteria, which is emphasized in the curriculum, was not been made. Based on the results of this study, we discuss ways to improve self-assessments in science textbooks and implications for effective use of self-assessments.

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Poster Presentation : **EDU.P-425**

Chemistry Education

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Gifted science students’ perceptions of classes emphasizing observation and communication

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In this study, we investigated the perceptions of middle school science gifted students who participated in an inquiry class that emphasized observation and communication. The class was structured so that students continuously participated in observation and communication, and questions were asked about whether the observation and communication activities were helpful in carrying out the inquiry activities, and if so, what specific inquiry activities were helpful. Students gave four types of responses as to why they found the observation and communication activities helpful.

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Poster Presentation : **EDU.P-426**

Chemistry Education

Exhibition Hall 2 THU 11:00~13:00

Characteristics Analysis of Dynamic Models Produced Using Technology

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In this study, the purpose of model and the nature of model were analyzed by comparing dynamic models produced using technology with static models produced using pictures, texts, formulas, etc. The purpose of model and the nature of model were analyzed by dividing them into representational and explanatory aspects. For this purpose, 18 pre-service chemistry teachers in their third year of education university in Chungcheongbuk-do were asked to produce static models and dynamic models, respectively. As a result of the study, the purpose of creating models for both static models and dynamic models included more explanatory aspects rather than representational aspects. However, as a result of analyzing the nature of model, the static models contained less explanatory aspects than the representational aspects compared to the dynamic models. Through this, it was confirmed that in the static models, the purpose of model and the nature of model were inconsistent, but in the dynamic models, the purpose of model and the nature of model were consistent. Therefore, it is judged that dynamic model produced using technology can increase the possibility of matching the purpose of model and the nature of model than static model produced using pictures, texts, formulas, etc.

Poster Presentation : **ENVR.P-427**

Environmental Energy

Exhibition Hall 2 THU 11:00~13:00

Enhancing Photocatalytic Hydrogen Production: Transitioning from Type I to Type II Heterojunction with CdS@PbS Heterostructures

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Storing solar energy as hydrogen (H_2) offers advantages such as high energy density, easy transportability, and cost-effectiveness. Various methods exist for converting solar energy into H_2, with direct photocatalysis or photoelectrolysis of water emerging as a favorable approach due to its efficiency and simplicity. Among light-driven photocatalysts, CdS stands out for its favorable band gap and thermodynamic compatibility for proton reduction. In this study, we synthesized CdS@PbS heterostructures using the cation exchange method and examined their performance of the photocatalytic hydrogen evolution reaction (HER). The as prepared core shell nanoparticles were photocatalytically inactive and produced hydrogen negligibly because of the unfavourable type Ⅰ heterojunction. However, the photoinduced morphological change of the film-like PbS shell to quantum dots caused the transition from the type Ⅰ to the type Ⅱ heterojunction and consequently greatly improved the photocatalytic efficiency compared to CdS photocatalyst. These results suggest that CdS@PbS heterostructures serve as effective photocatalysts for hydrogen production utilizing solar energy.

Poster Presentation : **ENVR.P-428**

Environmental Energy

Exhibition Hall 2 THU 11:00~13:00

2M Phase W1-xMoxSe2 Alloy Nanosheets to Enhance Electrocatalytic Hydrogen Evolution Reaction

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The phase control of transition metal dichalcogenide (TMD) is an intriguing approach for tuning the electronic structure towards extensive applications. In this study, W1-xMoxSe2 alloy nanosheets were synthesized via a colloidal reaction at 200-340 C. The 2H-2M phase was controlled by the growth temperature and the concentration of Se precursor. The 2H-2M phase transition temperature decreases with increasing x. The Se enrichment elevates the phase transition temperature increases, more significantly at lower x. High-resolution scanning transmission electron microscopy images were used to identify the stacking sequence of the 2M phase. The Mo and W atoms mixed homogenously over entire composition range. First-principles calculations employing Se-rich models indicated that Se enrichment induces conversion to the 2M phase. The 2M phase alloy nanosheets exhibited the composition-dependent electrocatalytic performance in the hydrogen evolution reaction (HER). These results provide an appealing strategy for phase control of TMD catalysts.Keywords: WSe2-MoSe2 alloy nanosheets, 2H-2M phase control, Se enrichment, spin-polarized density functional theory, hydrogen evolution reaction.

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Environmental Energy
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(WNbV)Se2 and (MoWNbV)Se2 Alloy Nanosheets: Composition Control to Enhance Electrocatalytic Hydrogen Evolution Reaction

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Department of Advanced Materials Chemistry, Korea University, Korea

Alloying of transition metal dichalcogenides (TMDs) has the potential for altering the electronic structure of materials to suit electrochemical applications. Herein, we synthesized (WNbV)Se2 and (MoWNbV)Se2 nanosheets at various compositions via a colloidal reaction. The mole fraction of V atoms (xV) was successfully increased up to 0.8, producing a metallic phase that is highly durable against hydration. The atomic mixing of the ternary and quaternary alloys is more random than that of the constitutional binary alloys. Compared to binary alloying, ternary alloying more effectively enhanced the electrocatalytic activity for acidic hydrogen evolution reaction (HER). The HER performance increased upon increasing xV to 0.5, and thereafter, it declined at higher xV primarily owing to surface oxidation. The analysis of Gibbs free energy for H adsorption revealed that VSe2 contains favorable sites for H adsorption, which explained the composition-dependent HER. These results provide a pioneering strategy for designing multicomponent TMD catalysts that maximize the advantages of each component.Keywords: Transition metal dichalcogenide, (WNbV)Se2 ternary alloy, (MoWNbV)Se2 ternary alloy, atomic mixing, spin-polarized density functional theory, hydrogen evolution reaction

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Environmental Energy

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Alloying of ReS2 and VS2 Nanosheets Enhances Electrocatalytic Hydrogen Evolution Reaction

Junaid Ihsan, Juyeon Kim, Jeunghee Park*

Department of Advanced Materials Chemistry, Korea University, Korea

Modulating the electronic structure of transition metal dichalcogenides via alloying is challenging despite the additional potential applications. In this study, a solvothermal reaction was used to synthesize composition-tuned ReS2-VS2 (Re1-xVxS2) alloy nanosheets featuring an expanded interlayer distance. Increasing x induces a phase transition from the semiconducting 1T″ phase ReS2 to the metallic 3R-stacking 1T phase VS2. Alloying via homogeneous atomic mixing renders the nanosheets more metallic and with less oxidation than VS2. First-principles calculations consistently predict the 1T″-1T phase transition of the atomically mixed alloy structures. The calculation also suggests that ammonia/ammonium intercalation drives the 3R stacking of 1T phase VS2. The Re1-xVxS2 nanosheets at x = 0.3–0.8 exhibited enhanced electrocatalytic activity toward water-splitting hydrogen evolution reaction (HER) in an acid electrolyte. Density of states and Gibbs free energy calculations showed that alloying increased the metallicity and thus effectively activated the basal S atoms toward the HER, supporting the observed increased HER performance of the alloy nanosheets.Keywords: Transition metal dichalcogenide, ReS2-VS2 alloys, phase transition, first-principles calculations, hydrogen evolution reaction

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Environmental Energy

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ReS2-MoS2-VS2 Ternary Aloy Nanosheets with Enhanced Electrocatalytic Hydrogen Evolution Reaction

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High-entropy alloy of transition metal dichalcogenides (TMDs) is a promising material for electrocatalytic water-splitting hydrogen evolution reaction. In the present study, a solvothermal reaction was used to synthesize composition-tuned ReS2-MoS2-VS2 (= (ReMo)1-xVxS2) alloy nanosheets featured with an expanded interlayer distance. The ternary alloying occurs with homogeneous mixing at an atomic scale. Alloying of 1T□ phase MoS2 with Re1-xVxS2 produces more metallic with less oxidation. The ternary nanosheets exhibit higher enhanced electrocatalytic activity toward acidic hydrogen evolution reaction (HER) than the ReS2-VS2 binary nanosheets. The enhancement is most prominent at xV = 0.7. First-principles calculations predict consistently the more metallic phase transition of the ternary alloy structures than the ReS2-VS2. Gibbs free energy (□ GH*) calculations showed that ternary alloying effectively activates the basal S atoms toward HER, supporting the enhanced HER performance of alloy nanosheets. Keywords: Transition metal dichalcogenide, ReS2-MoS2-VS2 alloys, solvothermal reaction, comosition control, hydrogen evolution reaction

Poster Presentation : **ENVR.P-432**
Environmental Energy
Exhibition Hall 2 THU 11:00~13:00

Application of Mechanochemically Synthesized Piezo-photocatalytic MoS2 Supramolecular Heterostructure for Ecofriendly Energy Production and Chemical Conversion

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The environmentally friendly green energy system which is able to respond to any external stimulus and participate in various chemical reaction can show significant advantages in terms of stable performance, versatility, and economic demand in the industrial society. However, the design of the economical and versatile high-performance catalyst system which is also advantageous for mass production is a notable challenge for the upcoming sustainable society. Here, we showed a productive and mechanochemical top-down fabrication strategy of molybdenum disulfide (MoS2) piezo-photocatalytic heterostructure with cyclic oligosaccharide and fullerene which aid both the exfoliation process and interfacial hydrophilicity through the self-assembly mechanism. Due to the electrochemical linkage and superior catalytic potential of each heterostructure component, the MoS2 heterostructure via mechanochemical synthesis could show the significant catalytic performances at various chemical conversion system such as hydrogen evolution, aniline production, and chemical dehalogenation process under the continuous exposure to various kinds of stimuli such as visible light, ultrasonic wave, and thermal treatment. Through this demonstration of MoS2 heterostructure system, we proved the feasibility and practicality of the application of supramolecular chemistry to a mechanochemical top-down manufacturing approach for transition metal dichalcogenide (TMD)-based catalysis systems.

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Flower-like heterostructure g-C3N4@NiO catalysts for efficient photodegradation of tetracycline and chlorpyrifos

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Nickel Oxide (NiO), as a typical p-type semiconductor, effectively mitigates the recombination of photogenerated electrons and holes at the interface with n-type semiconductors. As a result, NiO is a suitable catalyst for the formation of a graphitic carbon nitride (g-C3N4) heterojunction for the enhancement of the oxidation of organic pollutants. In this study, we synthesized a flower-like g-C3N4/NiO catalyst by combining g-C3N4 and NiO semiconductors to significantly enhance the photocatalytic performance. The surface porous structure was designed to increase the exposed surface area, thereby promoting pollutant adsorption and providing more active sites for pollutant decomposition. The target pollutants selected for investigation were tetracycline and chlorpyrifos. The resulting flower-like g-C3N4/NiO photocatalyst exhibited a flower-like structure with an expanded surface area and generated an electric field at the interface between g-C3N4 and NiO. This structure feature effectively attenuated the recombination of photogenerated electrons and holes.

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Poster Presentation : **ENVR.P-434**

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Titanium dioxide@Multi-walled carbon nanotubes Electrospun nanofiber mats for enhanced Cr(VI) photoreduction

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The most widely used photocatalyst, titanium dioxide (TiO2), has excellent stability, low cost, and strong oxidizing power, but its efficiency in visible light is limited. To overcome these limitations and improve the photocatalytic efficiency to control the area, a composite photocatalyst was prepared by incorporating multi-walled carbon nanotubes (MWCNTs) into pristine TiO2 synthesized by electrospinning with poly(vinylpyrrolidone). The presence of multi-walled carbon nanotubes (MWCNTs) promotes enhancement of the specific surface area, increases photocatalytic active sites, controls band gap, and prevents electron-hole recombination. The investigation and quantification of chromium(VI) decomposition efficiency revealed that the decomposition rate increased with higher MWCNT content. In conclusion, the incorporation of MWCNTs is related to the adsorption of harmful substances, the control of the band gap of TiO2, it improves the photoreduction efficiency due to the nanofiber structure produced by electrospinning.

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Poster Presentation : **ENVR.P-435**
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Electrochemical CO_2 reduction over surface-treated Au/TiO_2 electrodes

<u>Soyoung Kim</u>, Seon Young Hwang, Soo Yeon Bae, Yunji Gwon, Gaeun Yun[1], Choong Kyun Rhee[2], Youngku Sohn[2,*]

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Titanium dioxide emerges as a crucial material in terms of green technology. A surface-treated method of titanium dioxide (TiO_2) was presented in this work, followed by conducting electrochemical (EC) CO_2 reduction with the produced electrodes. It was observed that formate, CO, and C2-7 hydrocarbons were produced through the CO_2 reduction in our results. Depending on the thickness of Au deposition, the results of the products were primarily examined. Furthermore, we discovered an electrochemically-induced surface reaction that mimics the Fishcer-Tropsch (F-T) synthesis, resulting in the formation of long-chain hydrocarbons through C-C coupling/polymerization. These findings expands our understanding of catalytic performance in CO_2 reduction.

Poster Presentation : **ENVR.P-436**

Environmental Energy

Exhibition Hall 2 THU 11:00~13:00

Synthesis of porous expanded graphite using piranha solution for high-performance storage and hydrogen adsorption.

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Hydrogen energy is one of the essential technologies to achieve the global goal of net zero. However, in order to use hydrogen, storage technologies are needed. Hydrogen has the highest energy per mass of any fuel. Still, its low energy per unit volume due to its low ambient temperature density requires the development of advanced storage methods to achieve higher energy density. There are many different hydrogen storage methods, especially adsorption storage, which has become a promising candidate for storing hydrogen because of its excellent reversibility, fast kinetics, low energy consumption, and low cost. In this study, a physical storage method is used. As an adsorbent, graphite, which has excellent chemical stability, low mass density, high specific surface area, low cost, and eco-friendly material, is expanded using Piranha solution. Then, we report the changes in porosity and hydrogen adsorption capacity according to the degree of expansion and discuss the need for further research.

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Cu based electrochemical catalyst for ammonia synthesis

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The electrochemical method of recycling nitrogen pollutants into ammonia is gaining importance not only for the removal of environmental pollutants but also for reducing carbon emissions from conventional ammonia synthesis methods. This is emerging as crucial from an environmental perspective. We compared the faradaic efficiency of ammonia production under various conditions using Cu-based catalysts. Furthermore, we conducted an examination of the surface elemental oxidation states using X-ray photoelectron spectroscopy.

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April 24(Wed)~26(Fri), 2024, Suwon Convension Center, Korea

Poster Presentation : **ENVR.P-438**

Environmental Energy

Exhibition Hall 2 THU 11:00~13:00

Manufacture of carbon nanotube(CNTs) and chitosan nano-composite materials for gas adsorbents

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Carbon nanotube-based aerogels attract attention due to the high surface area and porosity. In this study, carbon nanotube aerogels were synthesized by carbon nanotubes and chitosan. Chitosan and CNT was dissolved in 1M HCl solution. The Chitosan/CNT mixture were freeze dry for preparing aerogels. Aerogels were carbonized at 200℃, 1 hr, and N_2 flow conditions. After carbonized, prepared samples were washed using water and ethanol until neutralization. The structural information of the activated carbons was measured by X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM). The 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).

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Poster Presentation : **ENVR.P-439**
Environmental Energy
Exhibition Hall 2 THU 11:00~13:00

Unique Surface modification of Pt/Cu for Electrochemical CO_2 Conversion

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Catalysts composed of platinum and copper exhibit heightened interactions, enabling them to function as activated catalyst. Specifically, electrochemical CO_2 conversion resulted in an enhanced selectivity towards H_2 and formate, driven by electrochemical mechanisms. In this study, we aimed to promote the production of major gas and liquid products by the surface treatment method. We investigated how the employed surface treatment techniques modify the size, shape and surface structure of catalyst nanoparticles and explore how these characteristics may influence the catalyst's activity and selectivity. Additionally, we examined the fundamental properties of the electrode using scanning electron microscopy, X-ray photoelectron spectroscopy, and energy dispersive X-ray spectroscopy.

Poster Presentation : **ENVR.P-440**
Environmental Energy
Exhibition Hall 2 THU 11:00~13:00

Role of Metallic Elements in Electrochemically Treated CuNiZn for Electrochemical CO_2 Reduction

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The electrochemical reduction of carbon dioxide(CO_2) has garnered significant attention as a promising approach to mitigate the adverse effects of greenhouse gas emissions. Designing effective and discriminating electrocatalysts is crucial for such processes. In this study, the CuNiZn electrode underwent various pre-treatments, including amperometry at positive oxidation potentials and linear sweep voltammetry towards positive potentials. We examined CO_2 electrochemical reduction at −2.2 $V_{Hg/HgO}$ in a highly alkaline solution using a potentiostat-equipped three-electrode cell. The primary reduction products, including H_2, CO, CH_4, C_{2+} hydrocarbons and formate were identified. Characterization techniques include X-ray photoelectron spectroscopy and energy-dispersive X-ray spectroscopy. These findings provide enhanced insights into C-C coupling, reduction products, and the distinct role played by each metal element in alloys during EC CO_2R.

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Poster Presentation : **ENVR.P-441**
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Interface engineering of TMDs and CoP heterostructure on carbon cloth for efficient hydrogen evolution reaction

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2D transition metal dichalcogenides (TMDs) are known as alternative electrocatalysts for hydrogen production due to their high catalytic activity, low cost, and easy preparation. Recently, transition metal phosphides (TMPs) are efficient semiconductor materials in hydrogen evolution reaction(HER) and desulfurization (HDS) which have high stability and electrically conductivity due to their low bandgap. Especially Co-based phosphides have been widely used in the HER due to their highest activity among the TMPs. However, the still limited catalytic activity compared to precious metal electrocatalysts in alkaline condition means that the development of new catalysts is needed. This work reports the possibility of designing novel and efficient HER catalysts by combining the promising CoP and TMDs. Also, Carbon cloth substrate takes advantage of high catalytic activity of TMDs with high conductivity, flexible surface. Herein, we synthesized a novel HER hybrid catalyst that is constructed by simple growth of TMDs and CoP on the surface of Carbon cloth. The synthesized TMD-CoP on the carbon cloth required low overpotential 68.2mV at 10mA cm-2 in 1.0M KOH and showed 74mV/dec Tafel slope value. These results show that the synthesized catalyst has almost similar performance to Pt. The synergistic effect between CoP and TMDs contributes significantly to improve the catalytic activity of HER. The Co and P, which occurred redistribution of electrons when combined with TMDs, acts as better hydride-acceptor and proton acceptor, respectively. This study provides a novel strategy for the design of non-precious metal electrocatalysts combined with improved HER performance.

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Exhibition Hall 2 THU 11:00~13:00

Solar liquid fuel production by using Mo-doped BiVO4 as photoanode and multilayered CuNi alloy/N-doped reduced graphene oxide/nafion as dark cathode

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The abatement of increased CO2 levels in the atmosphere is of great concern to improve the climate quality. On the other hand, the production of valuable chemicals from the renewable energy sources (solar and wind) is of paramount interest. In this regard, the solar liquid fuel (such as methanol and ethanol) production from the photoelectrochemical (PEC) CO2 reduction evolved as a sustainable and promising method. However, the solar to fuel conversion is hugely dependent on the efficient photoanodes which can produce high currents upon light illumination, and the dark cathodes which can selectively produce the liquid products. In this work, we attempted to develop Mo-doped BiVO4 photoanode and CuNi alloy/N-rGO/nafion dark cathode system to produce the methanol and ethanol selectively. The incorporation of Molybdenum (Mo-) into BiVO4 is expected to increase the photocurrent density by increasing the absorption co-efficient and by decreasing the recombination rate of the charge carriers. Meanwhile, the individual component in the multilayer cathode has a specific role for selective product formation. The CuNi alloy can selectively produce an important ‘CO’ intermediate during the CO2 reduction reaction, the N-doped reduced graphene oxide (N-rGO) is beneficial for the multielectron shuttling and CO2 adsorption/ activation, and the nafion layer promotes the proton migration. With the aid of multi proton/electron shuttling, the produced ‘CO’ intermediate over the CuNi alloy will eventually produce the solar liquid products. The electrodes fabrication procedure and their physical characterization results will be presented during the conference.

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Fe&Cu dual single atoms decorated N&S co-doped porous 2D Carbon Nanosheets/1D g-C3N4 hollow nanotubes heterojunction composite for enhanced photocatalytic CO2 reduction into solar liquid fuels

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Artificial photosynthesis i.e. photocatalytic reduction of CO2 into fuels or valuable chemicals, provides a promising solution to the challenges of global warming and energy supply. The development of an efficient artificial photosynthesis system requires a photocatalyst with a wide absorption range (from UV to near-IR region), high charge separation efficiency, strong redox capability, and high CO2 capturing and activation ability. Tremendous efforts have been devoted to developing efficient and stable photocatalysts for CO2 reduction, unfortunately, most of the semiconductor-based photocatalysts are not suitable for the large-scale and continuous flow CO2 reduction. Thus, the development of an efficient, stable, and cost-effective semiconductor-based photocatalyst for CO2 reduction is an essential requirement for future large-scale commercialization. The present work reports, the successful synthesis of Fe and Cu dual single atoms decorated N&S co-doped Carbon/g-C3N4 composite catalysts (Fe&Cu DSAs/N&S-Carbon/g-CN) by a simple thermal polycondensation followed by impregnation method. The prepared photocatalysts were systematically characterized by using various techniques. The atomic-level local geometric structure of Fe and Cu dual single atoms were investigated by X-ray absorption fine structure spectroscopy (EXAFS). The crystal structure and structural properties were characterized by X-ray diffraction (XRD), attenuated total reflectance-infrared spectroscopy (ATR-IR), and Raman spectroscopy. The optical properties and absorption characteristics of the synthesized photocatalysts were characterized by Ultraviolet-visible diffuse reflectance spectroscopy (UV-Vis DRS). The size, shape, and surface morphology of the synthesized photocatalysts were investigated by Field emission-scanning

electron microscopy (FE-SEM) and high-resolution transmission electron microscopy (HR-TEM). The surface elemental composition and chemical states of the elements were determined by High performance-X ray photoelectron spectroscopy (HR-XPS). Additionally, the life-time of photogenerated charge carriers were investigated by time resolved photoluminescence (TR-PL) and steady state photoluminescence (PL) spectroscopies. The photocatalytic CO2 reduction reaction (PC CO2RR) is currently under progress, and the results will be reported in the conference.

Poster Presentation : **ENVR.P-444**

Environmental Energy

Exhibition Hall 2 THU 11:00~13:00

Preparation of colloidal ZnTe/g-C3N4 quantum dots based efficient photocathode for photoelectrochemical reduction of CO2 into solar liquid fuels

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One of the most environmentally friendly ways to combat climate change is to employ renewable energy sources to cut carbon emissions. Photoelectrochemical CO2 reduction offers promising ways for converting CO2 into value-added fuels and chemicals using solar energy. The photoelectrochemical CO2 conversion to C2 products are more advantageous due to its greater energy density and higher commercial value over their C1 counterparts. The present work is focussed on the preparation of novel ZnTe/g-C3N4 quantum dots based photocathode for better selectivity towards C2 products. The ZnTe/g-C3N4 quantum dots based photocathode exhibits significantly improved photoelectrochemical performance compared to pristine ZnTe and g-C3N4. The synergistic effect between ZnTe and g-C3N4 quantum dots facilitated efficient charge separation and transfer, leading to enhanced photoelectrochemical CO2 reduction activity. The products derived from ZnTe-based photocathode are primarily to be the C1 products (mainly CO) with severe competition of hydrogen evolution reaction. Therefore, it is necessary for ZnTe to design a heterojunction to improve charge separation and selectivity of C2 products. The developed ZnTe/g-C3N4 quantum dots based photocathode holds great promise for efficient and selective photoelectrochemical CO2 reduction, offering a sustainable approach towards renewable fuel production and CO2 mitigation.